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A new holistic and integrated tool for the eco-design of industrial processes

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A new holistic and integrated tool for the eco-design of industrial processes

PhD Thesis

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Certificado

Prof. Dr. Javier Dufour Andía, Jefe de la Unidad de Análisis de Sistemas del Instituto IMDEA Energía y Catedrático de Universidad del Departamento de Tecnología Química, Energética y Mecánica de la Universidad Rey Juan Carlos, y **Dr. José Luis Gálvez Martos**, Investigador y Gestor de Proyectos en Tecnalia Research and Innovation

certifican

que **D. Miguel García Casas** ha realizado bajo su dirección y en las instalaciones de la empresa Contactica S.L., la Universidad Rey Juan Carlos y el Instituto IMDEA Energía la presente tesis doctoral titulada:

A new holistic and integrated tool for the eco-design of industrial processes

La presente tesis ha cumplido con los objetivos planteados, proporcionando resultados innovadores y originales. Por lo tanto, se expresa su conformidad para proceder a la defensa pública de la tesis para optar al grado de Doctor.

Fdo. Prof. Dr. Javier Dufour Andía Fdo. Dr. José Luis Gálvez Martos

Madrid, a 13 de noviembre de 2023

Foreword

This thesis has been released during my time as an industrial PhD researcher at Contactica S.L. and with the collaboration of the Systems Analysis Group at IMDEA Energy and the Rey Juan Carlos University. The project was partially founded by the Community of Madrid via the grants for the completion of industrial doctorates (Project reference: IND2017/AMB7644).

I would like to thank everyone that fueled my motivation during these years. From my directors and colleagues to my family, close friends, and partner. Keeping that fire burning has not always been easy. Without you all, there is no doubt it would have extinguished.

Synopsis

The primary motivation for this research is to develop a unique methodology and tool that combines process simulation, life cycle assessment (LCA), and life cycle costing (LCC) methodologies for the holistic application in the sustainability-based optimization of industrial processes. The eco-design framework and eco2des tool are created to address the challenges of incorporating and standardizing sustainability in the industrial sector in order to meet the increasing concern among different stakeholders, including policymakers, around sustainability.

The thesis begins with a state-of-the-art review exploring the integration of techno-economic analysis (TEA), LCC, LCA, and multiple criteria decision analysis (MCDA) methodologies for the eco-design of industrial processes. It then introduces the eco-design framework for industrial processes, which unifies existing standards and methods while addressing challenges in comparing environmental impacts and costs, maintaining consistent data sources, and reducing trial-and-error phases during technology upscaling. Furthermore, the eco2des tool is developed to encapsulate the eco-design framework, enabling users to evaluate the environmental impact, economic performance, and trade-offs of various process alternatives, offering a holistic approach to eco-design.

Two case studies validate the proposed methodological framework and tool, showcasing the versatility and potential of eco2des in providing sustainable designs and reliable insights on controversial technologies. The case studies underline the software's potential for holistic analysis without compromising implementation simplicity.

Challenges encountered during the development of eco2des include the lack of a common data interface, which hinders interoperability. Future work should focus on integrating Social Life Cycle Assessment (S-LCA), developing real-time digital solutions leveraging real-time data for enhanced decision-making, and exploring AI-driven predictive models based on neural network to produce the predictive life cycle inventory (P-LCI).

Overall, the novel eco-design methodology for industrial processes demonstrates its ability to generate optimal scenarios in process engineering, focusing on sustainable criteria. The eco2des tool serves as an effective decision support system, emphasizing its potential for holistic eco-design studies and accelerating the sustainable time-to-market for novel industrial processes.

Sinopsis

La investigación expuesta en la presente tesis busca desarrollar una metodología y una herramienta integrada que combine la simulación de procesos, el análisis del ciclo de vida (ACV), el análisis de costes del ciclo de vida (ACCV). Esta combinación tiene como propósito brindar una perspectiva holística en la optimización de procesos industriales basada en criterios de sostenibilidad. En este contexto, se introduce el marco metodológico de ecodiseño y la herramienta denominada "eco2des", concebidos para responder a los retos actuales de incorporar y estandarizar prácticas sostenibles en el ámbito industrial. Esta necesidad surge debido a la creciente inquietud de distintos actores, incluyendo legisladores, alrededor del desarrollo de una industria sostenible.

La tesis se inicia con una revisión del estado del arte, indagando en la integración del análisis tecno-económico, ACV, ACCV y las metodologías de análisis de decisión multicriterio aplicadas al ecodiseño industrial. A esto le sigue la exposición del marco metodológico de ecodiseño, que amalgama estándares y métodos preexistentes y se enfrenta a retos como la comparativa de impactos ambientales y costes, la coherencia en fuentes de datos y la minimización de iteraciones durante el desarrollo tecnológico. Paralelamente, se presenta eco2des, un software que encapsula este marco y facilita la evaluación holística de alternativas de proceso desde perspectivas ambientales y económicas.

El valor y aplicabilidad del marco y la herramienta se ilustran mediante dos casos de estudio. Estos evidencian la versatilidad de eco2des al ofrecer soluciones de diseño sostenible y conclusiones robustas respecto a tecnologías emergentes, resaltando su capacidad de análisis integral manteniendo sencillez en su uso.

No obstante, el desarrollo de eco2des presentó desafíos, como la ausencia de una interfaz de datos estandarizada que complicó su interoperabilidad. Por otro lado, las futuras investigaciones deberían considerar la incorporación del análisis social del ciclo de vida (ASCV), el fomento de soluciones digitales en tiempo real para optimizar la toma de decisiones, y la exploración de modelos basados en inteligencia artificial para elaborar inventarios predictivos del ciclo de vida.

Concluyendo, el marco metodológico de ecodiseño propuesto se erige como una herramienta potente en la ingeniería de procesos con enfoque sostenible. Adicionalmente, eco2des se destaca como un software eficaz de apoyo en la toma de decisiones, potenciando la realización de estudios holísticos de ecodiseño y agilizando la introducción al mercado de innovadores procesos industriales orientados a la sostenibilidad.

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List of Abbreviations

ABC	Artificial bee colony
ACO	Ant colony optimization
aEP	Aquatic eutrophication potential
AGR	Acid gas removal
AHP	Analytic hierarchy process
AI	Artificial intelligence
ANN	Artificial neural networks
AP	Acidification potential
APC	Automatic process control
ASU	Air separation unit
ATR	Auto-thermal reforming
BTL	Biomass to liquid
CAPE	Computer assisted process engineering
CAPEX	Capital expenditure
CEPCI	Chemical engineering plant cost index
CF	Characterization factor
CFB	Circulating fluidized bed
CFP	Carbon footprint
CHP	Combined heat and power
CML	Centrum voor Milieukunde Leiden (Centre of environmental science at Leiden)
COM	Component object model
COVID19	Coronavirus disease 2019
CPU	Central processing unit
DE	Differential evolution
DEA	Data envelopment analysis
DMU	Decision-making unit
DSS	Decision support system
EAT	Earnings after taxes
EBIT	Earnings before interest and taxes
EBITDA	Earnings before interest, taxes and depreciation
EBT	Earnings before taxes
EC	European Commission
EC-JRC	European Commission-Joint Research Centre

EPLCA	European Platform on Life Cycle Assessment
EROI	Energy return on investment
ETEA	Environmental techno-economic assessment
EU	European Union
FD	Fossil depletion
FT	Fischer-Tropsch
FTE	Full-time employees
FU	Functional unit
GA	Genetic algorithm
GACO	Extended ant colony optimization
GAM	Generalized additive model
GHG	Greenhouse gas
GHGE	Greenhouse gas emissions
GHSV	Gas hourly space velocity
GLAD	Global Life Cycle Assessment data access
GREET	Greenhouse gases, regulated emissions, and energy use in transportation
GUI	Graphical user interface
GW	Global warming
GWP	Global warming potential
HC	Hydrocracking
HP	High pressure
HRSG	Heat recovery steam generator
HT	High temperature
HTL	Hydrothermal liquefaction
IBEA	Indicator-based evolutionary algorithm
IDAE	Instituto para la diversificación y ahorro de la energía (Institute for the diversification and saving of energy)
iDE	Self-adaptive differential evolution
IoT	Internet of Things
IPCC	Intergovernmental panel on climate change
IRR	Internal rate of return
ISBL	Inside battery limits
ISO	International organization for standardization
LCA	Life Cycle Assessment
LCC	Life Cycle Costing

LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCOP	Levelized cost of production
LCSA	Life Cycle Sustainability Assessment
LCT	Life Cycle Thinking
LHSV	Liquid hourly space velocity
LHV	Lower heating value
LT	Low temperature
MADM	Multi-attribute decision making
MCDA	Multiple criteria decision analysis
MDEA	Methyl di-ethanol amine
MEA	Mono ethanol amine
MEAD	Multi-objective evolutionary algorithm by decomposition
MHACO	Multi-objective hypervolume-based ant colony optimizer
MINLP	Mixed integer non-linear programming
MOEA/D	Multi-objective evolutionary algorithm based on decomposition
MOGA	Multi-objective genetic algorithms
MOMT	Multi-objective multi-technology
MOOP	Multi-objective optimization problem
MP	Medium pressure
NBS	National bureau of standards
NPV	Net present value
NRC	National research council
NRE	Non-renewable energy
NREL	National renewable energy laboratory
NSGA	Non-dominated sorting genetic algorithm
NSGA-II	Non-dominated sorting genetic algorithm 2
NSPSO	Non-dominated sorting particle swarm optimization
OEF	Organization environmental footprint
OPEX	Operating expenditure
OSBL	Outside battery limits
PA	Proximate analysis
PEF	Product environmental footprint

PM-LCA	Process modeling Life Cycle Assessment
POCP	Photochemical ozone creation potential
P-LCI	Predictive Life Cycle Inventory
PSA	Pressure swing adsorption
PSO	Particle swarm optimization
PtG	Power to gas
PWP	Potable water plant
RA	Resource assessment
RAM	Random access memory
REDII	Renewable energy directive 2
RI	Respiratory inorganics
S-LCA	Social Life Cycle Assessment
SMR	Stepwise multivariate regression
SNG	Synthetic natural gas
SPEA2	Strength pareto evolutionary algorithm 2
SQL	Structured query language
SRK	Soave-Redlich-Kwong
TEA	Techno-economic analysis
tEP	Terrestrial eutrophication potential
TM-LCA	Territorial metabolism Life Cycle Assessment
TOPSIS	Technique for order preference by similarity to ideal solution
TRL	Technology readiness level
UA	Ultimate analysis
UN	United Nations
UP	Unit process
USA (or US)	United States of America
VIKOR	Vlsekriterijumska Optimizacija I Kompromisno Resenje (Multi-criteria optimization and compromise solution)
WGS	Water gas shift
WRI	World Resources Institute

RESUMEN EN CASTELLANO

1. Motivación

En tiempos recientes, la sostenibilidad en la producción y el consumo se ha posicionado en el centro del interés de empresas, gobiernos y consumidores, todos persiguiendo un mejor desempeño ambiental, económico y social en la cadena de suministro (Mazzi 2020). El pensamiento de ciclo de vida (LCT, por sus siglas en inglés, life cycle thinking) se manifiesta como un pilar fundamental para incorporar la sostenibilidad en el panorama global, cubriendo desde la investigación hasta la formulación de legislación (Pennington et al. 2007).

Europa ha puesto énfasis en el LCT, aplicando enfoques similares en sus políticas. Desde la Regulación Ecolabel de 1992 (EC 1992) hasta el Green Deal en 2019 (CEC 2019), la UE establece su meta de alcanzar la neutralidad de carbono para 2050. Post pandemia de COVID19, el LCT ha orientado las políticas europeas en la distribución de fondos para la Recuperación y Resiliencia, alineados con la sostenibilidad (CEC 2020b; EC 2021).

El desafío inminente es integrar y homogeneizar la sostenibilidad en sectores cruciales para el avance sostenible. La industria, representando más del 20% del PIB de la UE y dando empleo a 35 millones de personas (CEC 2020a), es un pilar fundamental. Casi la mitad de las emisiones de gases de efecto invernadero y más del 90% del deterioro de la biodiversidad y estrés hídrico tienen origen industrial (CEC 2019). Adicionalmente, la producción y consumo de energía en este sector es responsable del 24% de las emisiones globales de gases de efecto invernadero (World Resources Institute 2022). Por ende, el sector industrial es esencial para lograr una sostenibilidad global, conciliando prosperidad social y una economía sin emisiones netas.

Por lo tanto, para lograr el ambicioso objetivo de descarbonizar el sector industrial en línea con las políticas de emisiones netas cero, se deben estudiar y desarrollar nuevas cadenas de valor, así como optimizar las actuales en términos de indicadores clave de sostenibilidad. Sin embargo, durante el desarrollo de procesos innovadores, la falta de datos industriales dificulta el análisis de sostenibilidad del ciclo de vida, generando numerosas fases de prueba y error, aumentando el tiempo de lanzamiento al mercado y los costes, y pudiendo resultar en soluciones no optimizadas o inviables en términos de sostenibilidad. Sin embargo, los modelos predictivos y las simulaciones de procesos pueden calcular, mediante relaciones fisicoquímicas, el comportamiento de una tecnología en desarrollo a escala industrial y formular escenarios de optimización ambiental o económica. Aunque la simulación de procesos y las metodologías de ACV y ACCV están bien estructuradas y hay software comercial especializado, no existen investigaciones actuales que las combinen de manera holística en una herramienta única para la optimización económica y ambiental de cualquier diseño de proceso industrial en investigación y/o desarrollo. Esta carencia es precisamente lo que da origen a la presente tesis.

2. Objetivos

La presente tesis busca sentar las bases para un marco metodológico de ecodiseño orientado a la optimización sostenible de procesos industriales. Esta optimización se busca al combinar de manera integral la simulación de procesos, el ACV, el ACCV y técnicas de optimización matemática. A su vez, esta metodología se plasma en un software para garantizar su fácil adopción en investigaciones y proyectos subsiguientes. Concretamente, los objetivos primordiales de la tesis comprenden:

- Revisar el estado del arte de aplicaciones y marcos metodológicos que combinan modelos predictivos y descriptivos con ACV, ACCV y análisis de decisión multicriterio.
- Definir un marco metodológico integrado para la optimización basada en criterios sostenibles de procesos industriales, cimentado en la simulación de procesos, el ACV, el ACCV y técnicas de optimización matemática.
- Desarrollar un software precomercial para la optimización, basada en criterios sostenibles, de procesos industriales, fundamentado en la metodología propuesta.
- Probar y validar tanto la metodología planteada como el software desarrollado.

3. Revisión del estado del arte

El capítulo que nos ocupa profundiza en el estudio del estado del arte en relación con la integración del análisis tecno-económico (TEA, por sus siglas en inglés, techno-economic analys*is*) y la simulación de procesos con el ACCV, el ACV y el análisis de decisión multicriterio (MCDA, por sus siglas en inglés, multicriteria decision analysis). Esta revisión subraya la potencialidad y adaptabilidad de este enfoque integrador en diversos ámbitos industriales. Entre estos, se destacan las rutas de producción de biocombustibles, la revalorización del dióxido de carbono y la gestión del tratamiento del agua, mostrando así la versatilidad de este enfoque para impulsar decisiones enfocadas en la sostenibilidad en sectores variados.

Dentro de los estudios analizados sobre la aplicación integrada, cabe destacar el trabajo de Wang et al. (2010), donde se articuló el TEA con el ACV para diseñar rutas de gasificación en biorrefinerías mediante una optimización multiobjetivo. Esta metodología esclareció los conflictos inherentes entre las dimensiones económicas y medioambientales en dicho contexto. En una línea similar, el Laboratorio Nacional de Energías Renovables de EE. UU. (NREL, National Renewable Energy Laboratory) empleó una integración del TEA y ACV para valorar la producción de diésel renovable derivado de lípidos algales, usando modelos como Aspen Plus y GREET para los respectivos análisis. Los resultados del estudio de Davis et al. (2013), aunque con ciertas incertidumbres, ofrecieron una base cuantitativa para ponderar avances y desafíos en la fabricación de biocombustibles a partir de algas.

En el ámbito de la revalorización del CO_2, el estudio de McCord et al. (2021) se sirvió de un enfoque MCDA, fusionando resultados de la integración TEA-ACV, para categorizar cuatro fuentes de energía renovable destinadas a la generación de metanol a partir de CO_2. Este análisis, que contempló múltiples indicadores tanto ambientales como tecno-económicos, evidenció cómo un análisis integrado puede fortalecer la toma de decisiones en la industria, incluso cuando se manejan numerosos subcriterios.

Para concluir con las aplicaciones de este tipo de análisis, cabe mencionar el aporte de Mery et al. (2013), quienes propusieron una metodología integradora en el ámbito de la producción de agua potable. En respuesta a los desafíos que este sector presenta, crearon EVALEAU, una herramienta que combina modelización de procesos y ACV. Posteriormente, Ahmadi y Tiruta-Barna (2015) enriquecieron esta herramienta con un módulo de optimización, demostrando su eficacia en una planta potabilizadora en operación, generando un conjunto de soluciones alternativas para minimizar los impactos ambientales, reducir los costes operativos y maximizar la calidad del agua producida.

En resumen, aunque se observa un marcado interés por la aplicación de herramientas integradas de TEA y ACV para la evaluación de tecnologías novedosas, la mayoría de estas aplicaciones siguen siendo sectoriales, mostrando un vacío en cuanto a la interoperabilidad en el vasto campo de la ingeniería de procesos. De este modo, a pesar de las ventajas que ofrece la integración del ACV y ACCV (incluyendo TEA) en la evaluación de la sostenibilidad, hay una notable falta de uniformidad en cuanto a criterios y metodologías empleadas. Esta situación lleva a la carencia de guías formales para escoger un procedimiento de integración idóneo para diferentes propósitos.

En este punto, la revisión del estado del arte se adentra en los marcos metodológicos que intentan unir estos conceptos para solventar la carencia anteriormente expuesta. Un ejemplo destacado es el marco Multi-Objetivo Multi-Tecnología (MOMT), descrito por Li, Feaster y Kohler en 2019. El MOMT integra aspectos del ACV en el TEA tradicional. Pese a su aplicabilidad en la evaluación de diversas tecnologías y su capacidad para realizar análisis sensibles, este marco no toma en cuenta toda la cadena de valor, limitándose a las emisiones directas. Por otro lado, Thomassen et al. (2019) propusieron el marco prospectivo de Evaluación Ambiental Tecno-Económica (ETEA, por sus siglas en inglés, Environmental and Techno-Economic Assessment). Este marco, que amalgama el TEA y el ACV, se adecúa a distintos niveles de madurez tecnológica. Mediante módulos específicos, el ETEA posibilita la optimización de procesos sin tener que calcular todas las alternativas de diseño. Al identificar áreas críticas en términos económicos y ambientales durante las etapas tempranas del desarrollo tecnológico, este marco orienta la investigación hacia la minimización de esos impactos y costes.

A pesar de estos avances, tras evaluar los marcos metodológicos, se deduce que todavía existe una desarmonización. Además, ninguno de los marcos existentes abarca todas las metodologías que se identifican como esenciales en la propuesta metodológica de ecodiseño para procesos industriales, que es el foco central de esta tesis.

Para concluir, queda claro que una metodología unificada sería sumamente beneficiosa para diseñadores de procesos industriales, ya que permitiría una evaluación conjunta de la viabilidad económica y ambiental, y también una optimización no solo en base a criterios tecno-económicos, sino que también en base a impactos ambientales. Sin embargo, aún se ha de investigar más para construir un marco metodológico y herramientas congruentes que respalden a desarrolladores tecnológicos y políticos, impulsando en última instancia la integración del ecodiseño en cualquier proceso industrial.

4. Materiales y métodos

4.1. Simulación de procesos

Para llevar a cabo la simulación de procesos, se emplea un enfoque secuencial que comprende cuatro fases fundamentales: análisis del problema, entrada de datos, ejecución y análisis de resultados (ver Figura1).

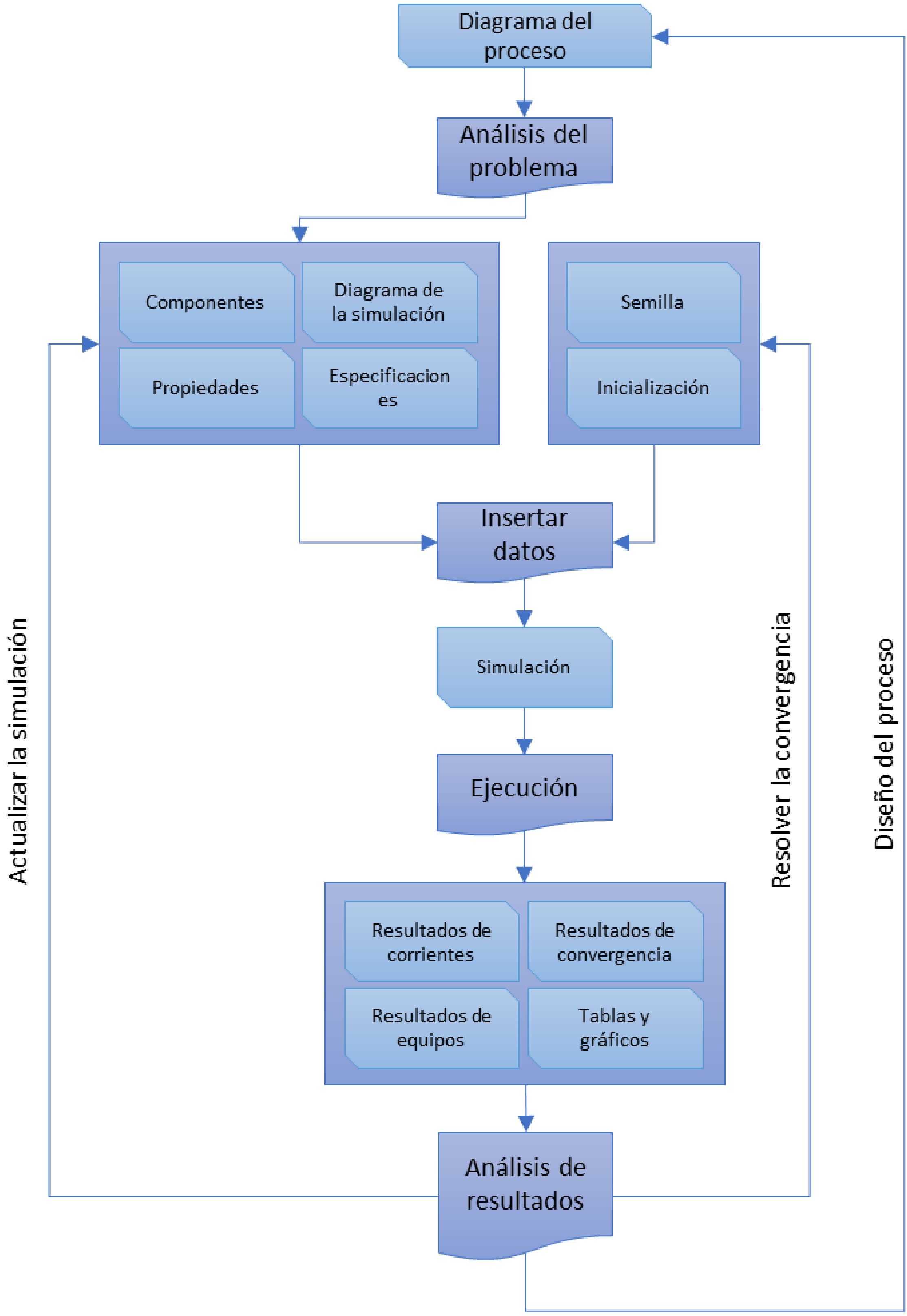

Figura 1. Enfoque de la simulación de procesos estacionarios (Basada en Dimian, Bildea, and Kiss 2014, 2)

- **Análisis del problema**: En esta etapa inicial, se realiza una adaptación del diagrama de flujo del proceso real en función de las capacidades del software utilizado y los objetivos planteados para la simulación. Es crucial comprender la química involucrada, seleccionar el modelo termodinámico adecuado y establecer los grados de libertad.

- **Entrada de datos**: Una vez analizado el problema, se procede a introducir los datos en el software de simulación. Estos datos provienen tanto del análisis previo del problema como de opciones de convergencia establecidas. En este paso se incluyen componentes, modelos termodinámicos, diagramas de flujo, corrientes de entrada y salida, y diversos parámetros relacionados con la convergencia.
- **Ejecución**: Durante esta fase, se corre la simulación para obtener diferentes resultados, como los balances de las corrientes y de los equipos, rendimientos y propiedades físicas.
- **Análisis de resultados**: Una vez obtenidos los resultados, es esencial validarlos. Si la simulación converge adecuadamente, se debe comprobar el equilibrio entre masa y energía, analizar las corrientes de recirculación y examinar las corrientes de los productos finales. Una vez validados estos aspectos, es posible llevar a cabo análisis más profundos, tales como análisis de sensibilidad y optimización de múltiples variables, para extraer más valor de los resultados del modelo.

Integrar la simulación de procesos en el enfoque metodológico del ecodiseño permite derivar de forma predictiva y descriptiva datos de inventario que serán útiles para modelos tanto ambientales como económicos. En este contexto, se ha optado por la “suite de ingeniería” Aspen ONE (AspenTech 2022b) como herramienta principal. Esta “suite” proporciona un sistema completo para la ingeniería de procesos asistida por computadora, abarcando desde sistemas de diagrama de flujo hasta paquetes especializados. En particular, Aspen Plus, que forma parte de esta suite, es una herramienta para ejecutar simulaciones en estado estacionario con una amplia base de datos y múltiples modelos termodinámicos. Es ampliamente utilizado en la industria para el diseño de procesos y análisis tecno-económicos. La elección de Aspen Plus para esta tesis se justifica por su versatilidad y aplicabilidad en campos como la ingeniería química, la producción de biocombustibles y el diseño de plantas de energía.

4.2. Análisis del ciclo de vida (ACV)

El Análisis del Ciclo de Vida (ACV) es una metodología estandarizada para evaluar las cargas ambientales de un producto, proceso o actividad a lo largo de su ciclo de vida. Sigue las normas internacionales 14040 y 14044 (ISO 2006a; 2006b) y comprende cuatro etapas principales (Figura 2).

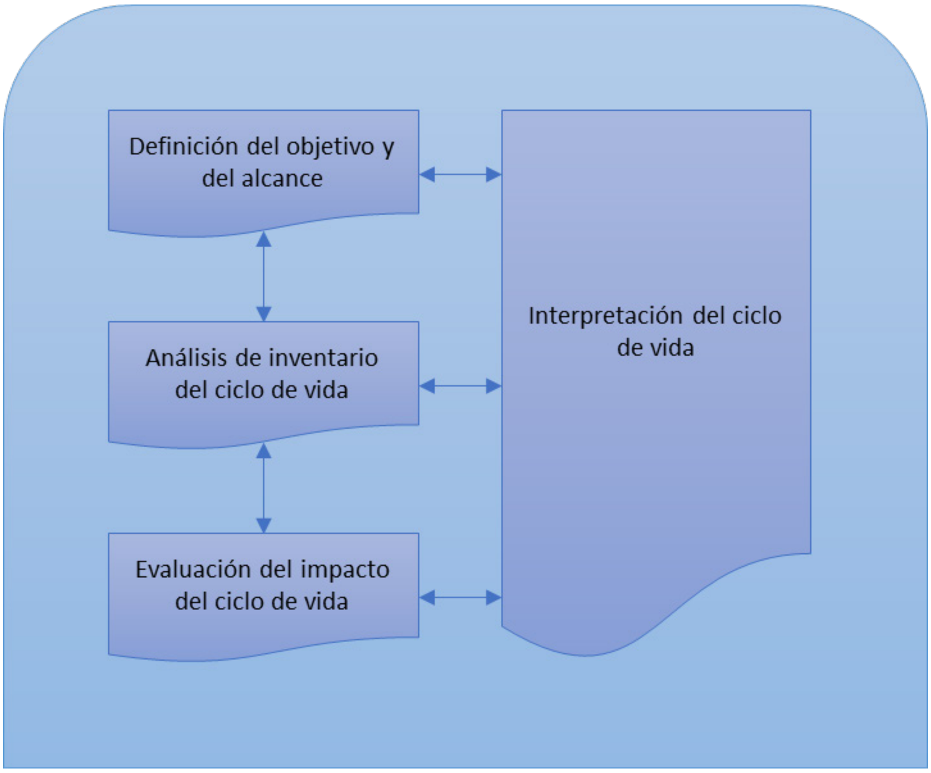

Figura 2. Marco metodológico del análisis del ciclo de vida (basado en ISO 2006b).

- **Definición del objetivo y del alcance**: En esta etapa se establece el propósito del estudio, se define la unidad funcional, se determinan los límites del sistema y se configuran otros parámetros metodológicos.
- **Análisis de inventario del ciclo de vida (ICV)**: Esta fase implica la recolección de datos que representan entradas y salidas del sistema. Aquí se aborda la multifuncionalidad y se determinan los procedimientos de asignación.
- **Evaluación del impacto del ciclo de vida (EICV)**: En esta etapa, los flujos medioambientales son clasificados en categorías de impacto. Dependiendo de las necesidades, pueden incluirse pasos de normalización y ponderación.

- **Interpretación del ciclo de vida**: Aquí se identifican los problemas más significativos del estudio, se evalúa su integridad, sensibilidad y consistencia, y se finaliza con la presentación de conclusiones, restricciones y recomendaciones.

Integrar el ACV en el marco metodológico de ecodiseño para procesos industriales permite a los investigadores analizar y potenciar el desempeño medioambiental a lo largo de todas sus fases. En términos de herramientas para realizar ACV, existen numerosas opciones de software, desde comerciales hasta de código abierto. La elección de una de estas herramientas se basa en diversos criterios, como funcionalidad, disponibilidad de bases de datos, interfaz, calidad de datos y principios de modelado. En este trabajo se optó por utilizar Brightway2 (Mutel 2017), un software de ACV de código abierto. La elección de esta herramienta se fundamentó en sus capacidades para realizar cálculos rápidos, la amplia disponibilidad de bases de datos medioambientales, su facilidad de integración en la herramienta de ecodiseño que se está desarrollando y su completo set de funciones, adecuado para las necesidades de la tesis.

4.3. Análisis de costes del ciclo de vida (ACCV)

El Análisis de Costes del Ciclo de Vida (ACCV) es una metodología orientada a la evaluación de los costes económicos asociados a un producto, proceso o actividad durante su ciclo de vida. La metodología se estructura en varias etapas fundamentales visibles en la Figura 3 y detalladas a continuación.

- **Definición del objetivo y del alcance**: Esta fase establece las metas del estudio, determina los límites del sistema, especifica los indicadores de desempeño económico y señala las fuentes de datos a consultar.
- **Recolección de datos**: En esta etapa se recaban los datos necesarios para la evaluación económica. Aquí se identifican indicadores de coste clave como el Valor Actual Neto (VAN), la Tasa Interna de Retorno (TIR) o el periodo de recuperación de la inversión.
- **Evaluación de costes**: Este paso se enfoca en calcular el coste de capital (CAPEX, por sus siglas en inglés, capital expenditures), que comprende el coste total de diseño, construcción e instalación del proceso, y el coste operativo (OPEX,

también en inglés, operational expenditures), que cubre los costes vinculados con la producción, tanto fijos como variables. Una vez recopilados estos datos, se elabora un modelo de flujo de efectivo que permita determinar los indicadores de desempeño económico previamente definidos.

- **Interpretación**: Esta fase tiene como finalidad identificar problemas críticos, evaluar la solidez, sensibilidad y coherencia de la información recolectada, y concluir con recomendaciones y restricciones para el estudio.

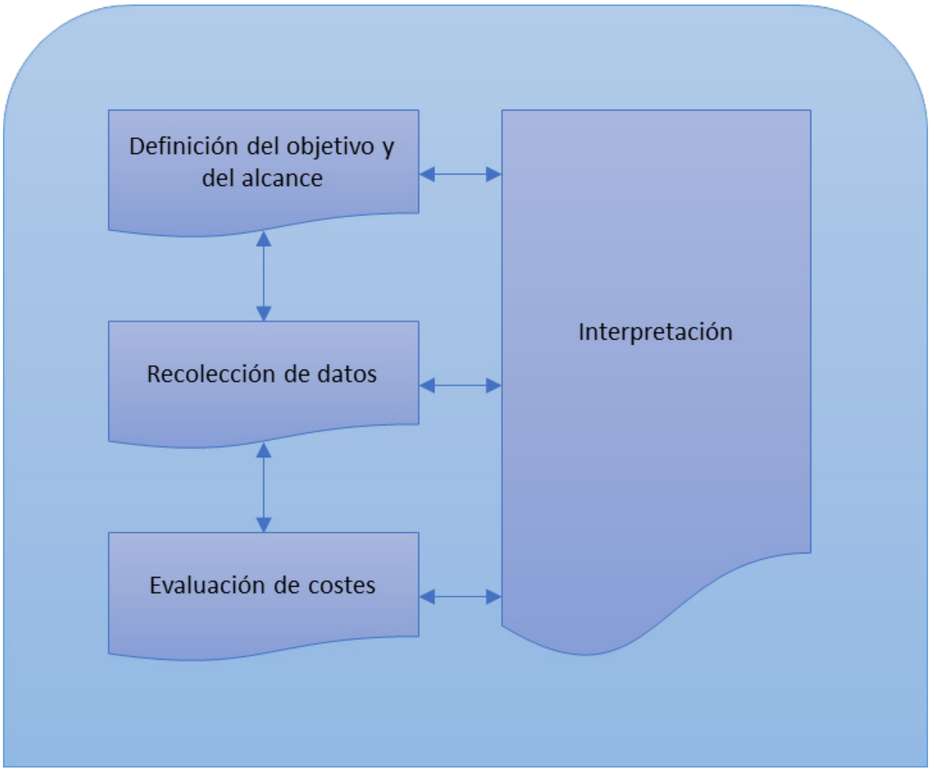

Figura 3. Marco metodológico del análisis de costes del ciclo de vida (basado en ISO 2006b).

La integración del ACCV convencional (es decir, aquel que no tiene en cuenta el coste de las externalidades) en el marco del ecodiseño permite analizar y optimizar el rendimiento económico de procesos industriales desde una perspectiva integral. En cuanto a herramientas para llevar a cabo el ACCV, existen diversas opciones en el mercado, siendo las hojas de cálculo de Excel una de las más utilizadas. Sin embargo, estas herramientas pueden presentar limitaciones en aspectos como flexibilidad para modelar o dificultades en la integración con otros sistemas. Es por esto que, para esta tesis, se optó por diseñar un programa específico de estimación de costes mediante el uso de Python (Python Software Foundation 2022), lo que permite una mayor adaptabilidad.

4.4. Optimización multiobjetivo

La optimización multiobjetivo surge como respuesta a problemas de optimización que presentan múltiples objetivos, a menudo en conflicto. A diferencia de la optimización mono-objetivo, donde se busca una única solución óptima, en la optimización multiobjetivo se aspira a encontrar un conjunto de soluciones, conocido como el frente de Pareto. Estas soluciones representan diferentes compromisos entre los objetivos y permiten a los responsables de la toma de decisiones escoger la solución que mejor se alinee con sus prioridades.

Un problema de optimización multiobjetivo puede formularse de la siguiente manera:

$$Minimizar: \quad F(x) = \{f_1(x), f_2(x), \dots, f_m(x)\}$$

$$Sujeto\ a: \quad x = [x_1, x_2, \dots, x_n] \in X$$

$$l_i \leq x_i \leq u_i \quad i = 1,2, \dots, n$$

$$g_i(x) \leq 0 \quad i = 1,2, \dots, p$$

$$h_i(x) = 0 \quad i = 1,2, \dots, q$$

Donde $F(x)$ es el vector objetivo m-dimensional, x es el vector de decisión n-dimensional y X es el espacio de decisión n-dimensional. Luego, g_i representa la i-ésima restricción de desigualdad y h_i representa la i-ésima restricción de igualdad. p y q son los números de restricciones de desigualdad e igualdad, respectivamente. Finalmente, l_i y u_i representan los límites inferior y superior de la i-ésima variable de decisión, respectivamente.

La metodología de optimización multiobjetivo comprende varios pasos fundamentales (Figura 4):

- **Análisis del problema**: Es crucial entender cuáles son los objetivos a optimizar, delimitar el espacio de decisión, identificar las funciones objetivo y las restricciones, así como realizar análisis de sensibilidad para entender el espacio de decisión.
- **Formulación del problema**: Una vez comprendido el problema, se formula matemáticamente como un problema de optimización multiobjetivo, considerando todas las variables de decisión, funciones objetivo y restricciones.
- **Selección del algoritmo**: Se debe escoger un algoritmo de optimización adecuado al problema en cuestión. Los algoritmos metaheurísticos suelen ser una buena elección para problemas multi-objetivo debido a su capacidad de explorar amplios espacios de búsqueda y tratar con complejidades inherentes a estos problemas.
- **Análisis de resultados**: Luego de obtener el frente de Pareto, es fundamental analizar las soluciones para comprender las relaciones entre las variables de decisión y los objetivos. Además, se deben evaluar el rendimiento y la eficiencia de los algoritmos utilizados para asegurar que se haya alcanzado una solución confiable.

Este es un proceso iterativo que ayuda a llegar a una solución fiable, la cual puede ser analizada en detalle utilizando métodos cualitativos y técnicas de visualización. Asimismo, los responsables en la toma de decisiones pueden seleccionar una solución de compromiso para un análisis exhaustivo de la misma.

La integración de la optimización multiobjetivo en el marco de ecodiseño brinda la posibilidad de analizar y comparar distintas soluciones óptimas. Esto se traduce en una mayor flexibilidad para tomar decisiones que beneficien tanto al medio ambiente como al aspecto económico de los procesos. En relación con la herramienta seleccionada para esta tesis, pygmo (Biscani and Izzo 2020), una librería de Python, se presenta como una excelente elección debido a su interfaz unificada para algoritmos y problemas de optimización, amplia gama de algoritmos de optimización disponibles y diseño orientado a objetos, lo que facilita la creación de clases personalizadas y su integración dentro de la herramienta de ecodiseño que se desarrolla en esta tesis.

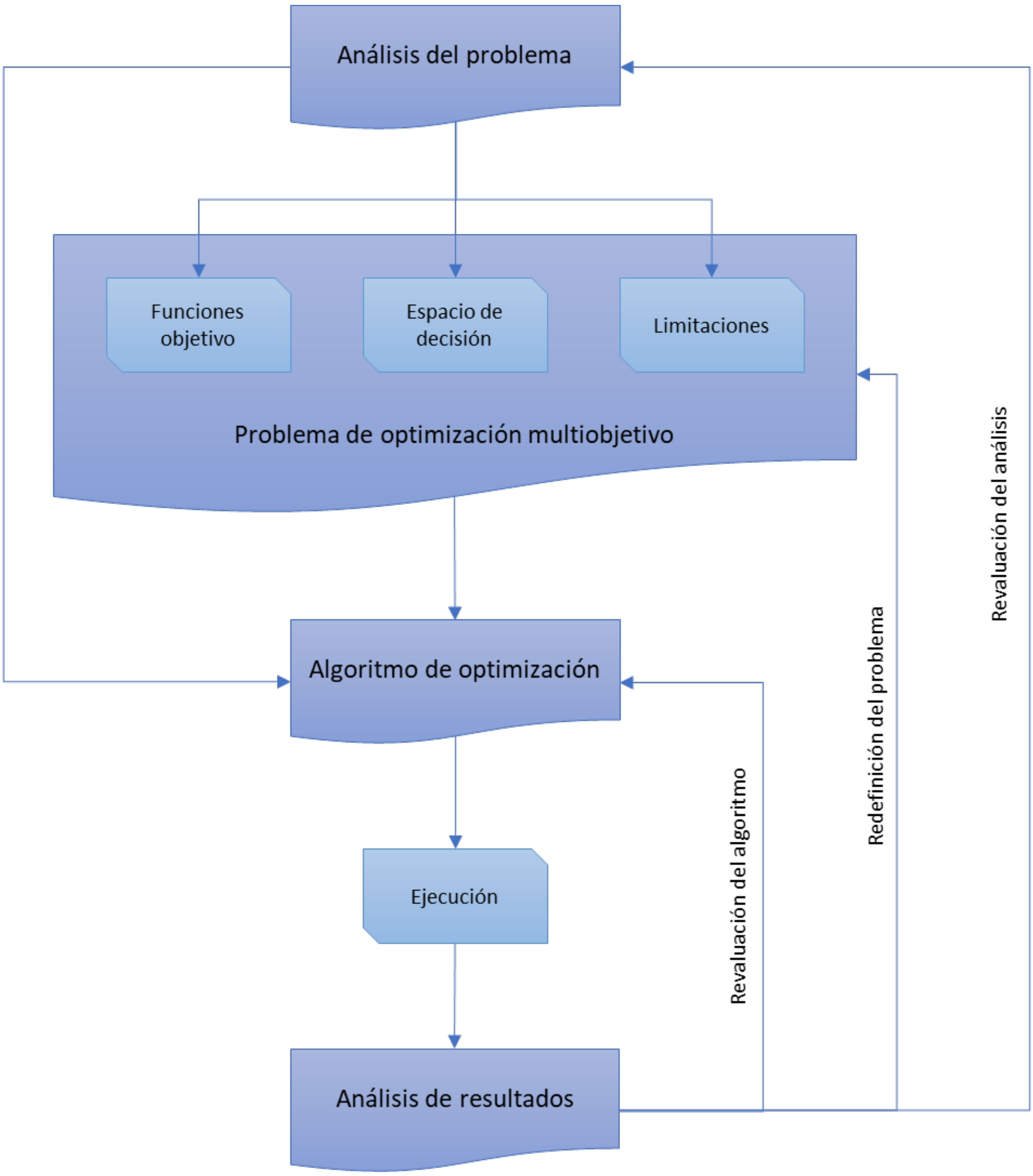

Figura 4. Enfoque de un problema de optimización multiobjetivo

5. Marco metodológico para el ecodiseño de procesos industriales

El marco metodológico se basa en metodologías de pensamiento del ciclo de vida y sus estándares existentes, así como en la adopción de los métodos de simulación de procesos y optimización multiobjetivo presentados anteriormente, con el objetivo principal de desarrollar una metodología holística para el ecodiseño de procesos industriales que combine simulación de procesos, ACV, ACCV y optimización multiobjetivo. Los principales pasos de este marco se muestran en la Figura 5.

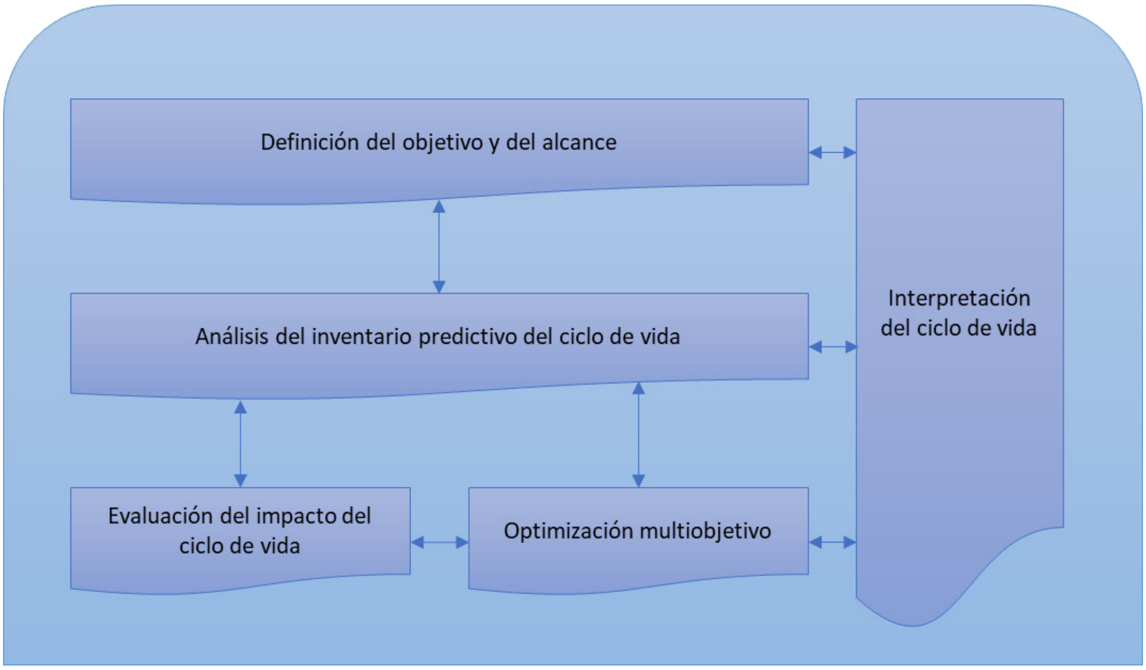

Figura 5. Marco metodológico para el ecodiseño de procesos industriales

5.1. Definición del objetivo y del alcance

El inicio de cualquier estudio orientado al ciclo de vida se encuentra en la precisa delimitación de su objetivo y alcance, fundamentales para garantizar la congruencia con la finalidad proyectada. Debido a la naturaleza iterativa de este proceso, el alcance puede ajustarse y afinarse conforme avanza el estudio. En el contexto de este marco, el propósito principal radica en la formulación de un diseño para procesos industriales que, a lo largo de todo su ciclo de vida, reduzca al máximo los impactos medioambientales y los costes, siempre respetando las restricciones tecnológicas inherentes.

Es indispensable que el alcance esboce con claridad elementos como el sistema de producto, la unidad funcional, los límites del sistema, los protocolos de asignación, la metodología correspondiente al ACV, los indicadores económicos relacionados con el ACCV, y aspectos relacionados con la optimización, como los objetivos, el espacio de decisión, las barreras del problema; y, por último, la interpretación de los resultados. También deben ser especificados los requisitos de calidad de los datos a utilizar, suposiciones, restricciones, revisiones críticas (si fuesen necesarias) y el formato de presentación del informe.

El sistema de producto engloba tanto los sistemas de primer plano como los de fondo. El sistema de primer plano se identifica con el proceso industrial per se, modelado a partir de relaciones fisicoquímicas y modelos predictivos; mientras que el sistema de fondo comprende el resto de los procesos de la cadena de valor cuyos costes e impactos ambientales se introducen en los diferentes análisis de ciclo de vida a través de bases de datos especializadas. Por otro lado, la definición de la Unidad Funcional (UF) es un elemento de vital importancia, dado que determina la función que el sistema de producto debe cumplir y sienta las bases para los modelos de ACV y ACCV. En paralelo, los límites del sistema establecen qué procesos unitarios se incluyen en el inventario del ciclo de vida y delimitan el rango de acción del estudio. En este marco metodológico, una estrategia de cuna a puerta resulta suficiente para optimizar los parámetros de diseño del proceso industrial. Aun así, se sugiere considerar una extensión hacia una perspectiva de cuna a tumba, post-optimización del proceso operativo, con el fin de obtener un análisis panorámico y completo, en particular de los impactos medioambientales.

En esta etapa también se identifican aquellas variables de diseño que tienen incidencia en la simulación del proceso, así como las variables topológicas, como la elección de tecnologías o insumos. Un análisis preliminar y un estudio de sensibilidad pueden ser instrumentos útiles para afinar el espacio de decisión en iteraciones subsiguientes. Es importante subrayar que las restricciones técnicas se establecen dentro de la simulación del proceso y son imprescindibles para la convergencia del modelo. Por otro lado, las restricciones de carácter ambiental y económico deben ser dialogadas y acordadas con las partes interesadas correspondientes, y posteriormente categorizadas en desigualdades e igualdades para su integración en el problema de optimización. Finalizando este paso, durante la clasificación de fuentes de datos, se determinan los resultados de la simulación necesarios para nutrir los modelos de ACV y ACCV generando el inventario predictivo.

5.2. Análisis del inventario predictivo del ciclo de vida (IPCV)

El análisis del Inventario Predictivo del Ciclo de Vida (IPCV) constituye un pilar esencial en el estudio de ecodiseño. Su rol principal es esbozar el protocolo para la recopilación de datos de inventario, asegurando al mismo tiempo su calidad y exactitud (Figura 6). De naturaleza iterativa, esta etapa involucra no solo al modelo de simulación del proceso, sino también al modelo de ACV, al modelo de ACCV y el problema de optimización. Esta interacción da como resultado un inventario predictivo y autodescriptivo, íntimamente ligado al proceso simulado que facilita las correcciones automáticas del inventario ante cambios en los datos de entrada de la simulación y posibilita su integración en una estructura de optimización.

Es fundamental coordinar de manera eficaz los protocolos de recolección de datos. Este esfuerzo abarca la identificación de los datos generados por la simulación que serán esenciales para los modelos ACV y ACCV, el discernimiento del origen de los objetivos de optimización, y el diseño de métodos que permitan la incorporación de variables de decisión a la simulación. Asimismo, se deben integrar restricciones técnicas a la simulación, al tiempo que se delimitan restricciones adicionales. La construcción de un modelo de simulación fiable es un reto que requiere de un trabajo iterativo. En este proceso, se consideran aspectos como los componentes, modelos termodinámicos, diagramas de flujo, corrientes de entrada, unidades de sistema y enfoques computacionales (Figura 7). Para garantizar su fiabilidad, el modelo debe ofrecer resultados que converjan dentro del espacio de decisión previamente delimitado para el problema de optimización, lo que podría implicar ajustes en dicho espacio o en el modelo en sí.

En el contexto del marco metodológico de ecodiseño aplicado a procesos industriales, el modelo de simulación sirve como fuente de datos de inventario. Así, cuando un nuevo vector de variables de decisión es evaluado, el inventario predictivo se crea resolviendo la simulación, proporcionando los datos necesarios para los modelos de ACV y de ACCV y entregando, en última instancia, los objetivos para la optimización que formarán parte de una nueva generación que será evolucionada en las subsecuentes iteraciones del algoritmo.

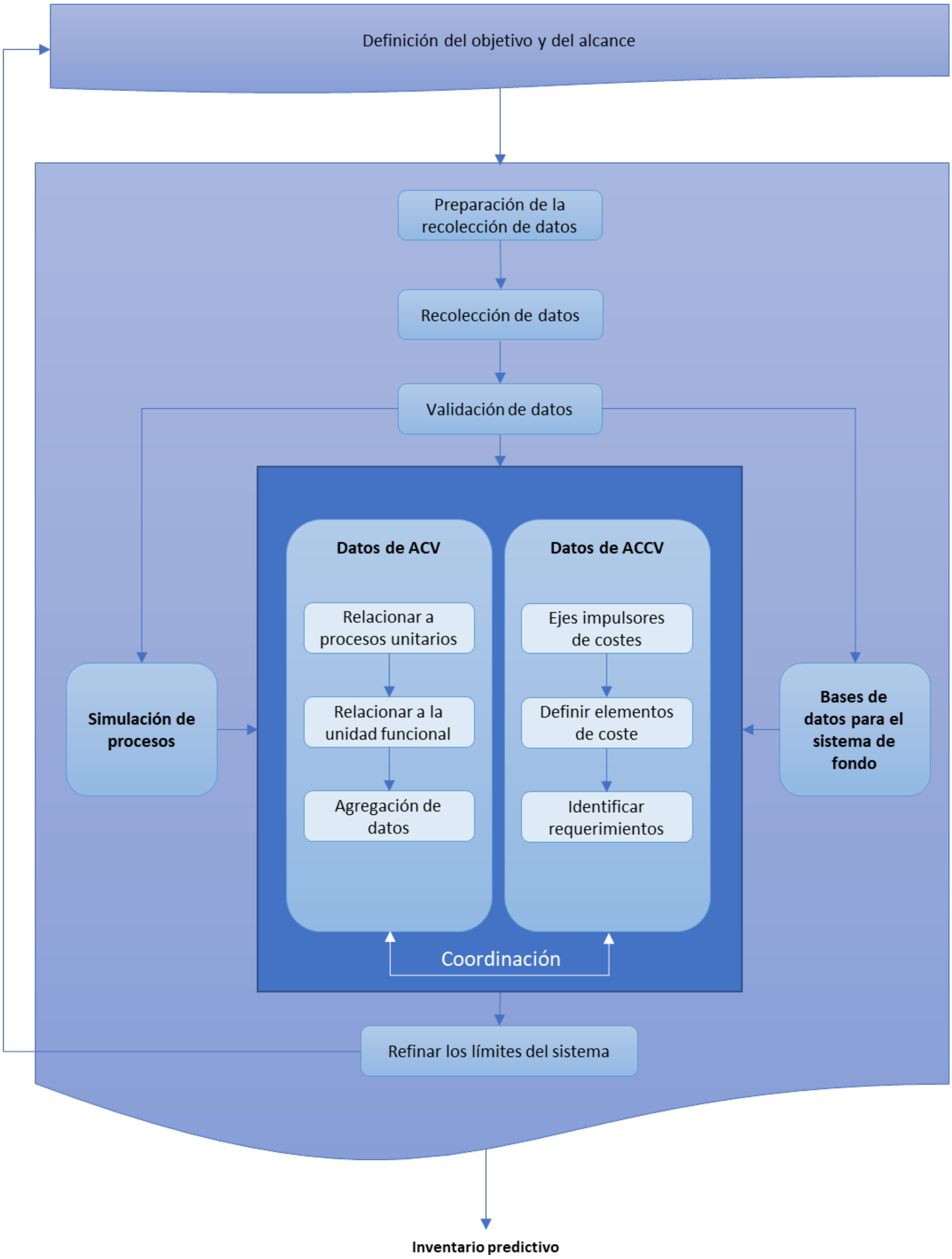

Figura 6. Análisis del inventario predictivo del ciclo de vida en el marco de ecodiseño para procesos industriales

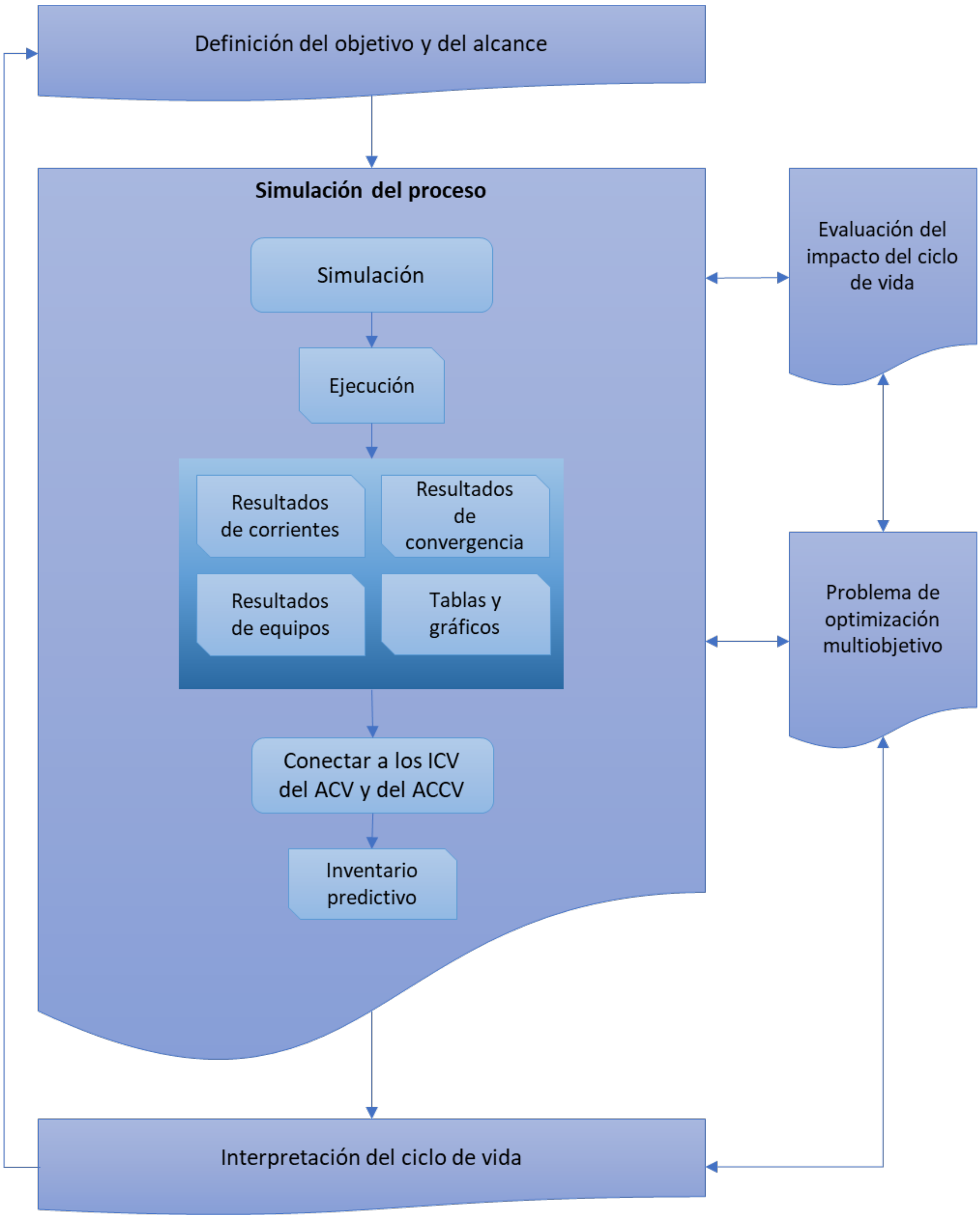

Figura 7. Simulación de procesos en el marco de ecodiseño para procesos industriales

5.3. Evaluación del impacto del ciclo de vida (EICV)

En la fase de Evaluación del Impacto del Ciclo de Vida (EICV), se da un tratamiento analítico a los datos del inventario predictivo, obtenidos en la etapa previa, con el fin de determinar los impactos tanto ambientales como económicos por medio de los modelos de ACV y ACCV.

Desde una perspectiva ambiental, los flujos generados son categorizados en distintas áreas de impacto. Estas categorías son esenciales, ya que posteriormente pueden convertirse en objetivos a considerar en el problema de optimización. Desde el punto de vista económico, aquellos datos del inventario predictivo que están vinculados a elementos con un coste directo son utilizados para determinar el coste de capital (CAPEX) y el coste operativo (OPEX) del sistema de producto en cuestión. A su vez, se elabora un modelo detallado de flujo de caja, que arroja indicadores adicionales de desempeño económico. Este análisis financiero es fundamental para comprender no solo la viabilidad económica del proceso, sino también para equilibrar los aspectos ambientales y económicos del ecodiseño.

5.4. Optimización multiobjetivo

La etapa de optimización multiobjetivo se estructura de manera coherente con las fases previas de análisis de inventario predictivo del ciclo de vida y evaluación del impacto del ciclo de vida, como se detalla en la Figura 8.

Dentro de este proceso, los objetivos específicos de optimización emergen a partir de los datos obtenidos en el inventario predictivo y de los resultados arrojados en la evaluación del impacto del ciclo de vida. El espacio de decisión, en este contexto, se esculpe a partir de los parámetros de diseño y las decisiones topológicas asumidas en los modelos de simulación y ciclo de vida. Es esencial mencionar que mientras las restricciones técnicas se integran de manera intrínseca en el modelo de simulación, existe la posibilidad de añadir restricciones adicionales directamente en el problema de optimización. Estas podrían surgir de las etapas previas del marco metodológico o de requerimientos específicos establecidos por las partes interesadas, como una rentabilidad mínima esperada por los accionistas.

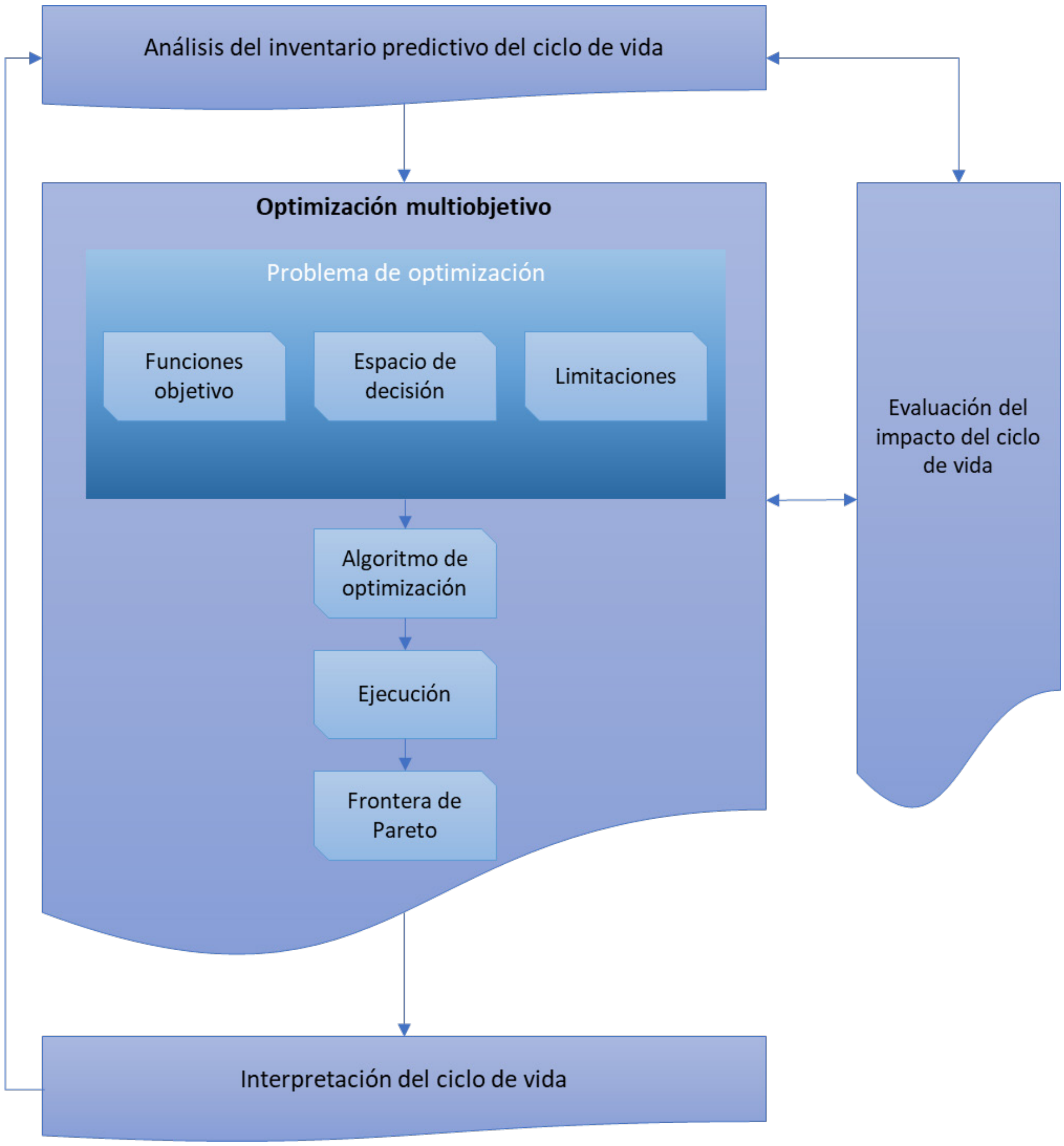

Figura 8. Optimización multiobjetivo en el marco de ecodiseño para procesos industriales

5.5. Interpretación

La interpretación es una fase clave que tiene por objetivo sintetizar y analizar de forma crítica la información obtenida. En ella se identifican y resaltan los aspectos más relevantes, se lleva a cabo una evaluación de los datos a través de controles de exhaustividad, sensibilidad y consistencia, y se elaboran conclusiones, limitaciones y recomendaciones pertinentes.

Uno de los principales propósitos de esta etapa es garantizar que los resultados del ecodiseño sean fiables y robustos. Es esencial presentar los hallazgos de una manera que facilite la comprensión y análisis por parte de los interesados. En este sentido, los controles de sensibilidad desempeñan un papel vital, ya que permiten evaluar la influencia de las incertidumbres presentes en los datos y ajustar el espacio de decisión, afinando así el proceso de simulación y asegurando una mayor fiabilidad en los modelos de ACV y ACCV.

Es importante subrayar que la integración de la optimización multiobjetivo dentro del marco metodológico facilita y enriquece la interpretación final, automatizando la evaluación de miles de escenarios óptimos. Este enfoque proporciona una perspectiva más amplia y detallada sobre los aspectos críticos del sistema y su rendimiento en términos de sostenibilidad, considerando las variaciones y condiciones específicas del proceso industrial en estudio.

6. Herramienta de ecodiseño para procesos industriales: eco2des

En el ámbito de la ingeniería de procesos, eco2des surge como una solución integral en respuesta a la creciente demanda de procesos sostenibles y decisiones basadas en datos. Ofrece a los ingenieros y profesionales relacionados una herramienta que combina precisión con velocidad, flexibilidad con robustez, y al mismo tiempo es escalable para adaptarse a los retos del futuro.

eco2des ha sido desarrollada en Python para la optimización de procesos industriales en base a criterios sostenibles y ofrece soluciones prometedoras a las demandas anteriormente expuestas. eco2des documenta los inventarios del ciclo de vida, caracterizándolos mediante el impacto ambiental y económico, mientras también utiliza modelos fisicoquímicos para la producción automática de datos de inventario, generando el inventario predictivo del ciclo de vida desarrollado en el marco metodológico de la presente tesis. Además, mediante la integración de la optimización multiobjetivo, eco2des permite automatizar y agilizar la toma de decisiones durante la fase de interpretación, ya que minimiza impactos ambientales y costes.

6.1. Arquitectura de eco2des

La arquitectura de eco2des, representada en la Figura 9, se construye en torno a principios de modularidad y mantenibilidad, utilizando el paradigma de la programación orientada a objetos para facilitar la expansión y la integración con otros sistemas y aplicaciones. Veamos más a fondo los módulos que la componen:

- **e2dprojects**: Este módulo administra la logística de los proyectos dentro de la herramienta. Un proyecto puede ser entendido como un contenedor para todas las entidades relevantes: desde la simulación de procesos y los modelos de ACV/ACCV, hasta la configuración del problema de optimización. Utiliza una base de datos SQLite (SQLite Consortium 2022) para almacenar y gestionar metadatos, aprovechando la eficiencia y portabilidad de esta base de datos.
- **e2dsimulation**: Este componente trabaja en estrecha colaboración con los archivos de simulación generados por Aspen Plus (AspenTech 2022a). Su tarea es navegar y manipular el árbol de datos, que comprende elementos como componentes, corrientes, equipos y unidades de proceso. Permite una interacción dinámica con la simulación, lo que es fundamental para ajustar y leer los parámetros críticos para la optimización.
- **e2dlca**: Este módulo es fundamental para evaluar los impactos ambientales. Utiliza Brightway2 (Mutel 2017), una herramienta reconocida en el ámbito del ACV, lo que garantiza precisión y confiabilidad en los cálculos. Asimismo, se encarga de gestionar los datos y proporciona herramientas para el análisis y visualización de los resultados. Por último, se destaca su capacidad para importar bases de datos de inventario extensas para ser usadas como sistemas de fondo y manejarlas eficientemente almacenando en caché la representación matricial de las mismas.
- **e2dlcc**: Es el complemento del módulo e2dlca, enfocado en la evaluación de costes del ciclo de vida, esencial para calcular indicadores financieros como el Valor Actual Neto (VAN) o la Tasa Interna de Retorno (TIR). Este módulo también

contribuye a la fase de interpretación, ofreciendo herramientas analíticas adicionales.

- **e2doptimization**: Constituye la interfaz para la formulación y solución de problemas de optimización multiobjetivo. Ofrece a los usuarios la posibilidad de definir variables de decisión, establecer límites y objetivos. El módulo proporciona varios algoritmos de optimización global heurísticos para uno o varios objetivos, heredados de la biblioteca pygmo (Biscani and Izzo 2020). Tras la resolución de los problemas, permite visualizar la frontera de Pareto y exportar los resultados para su análisis posterior.

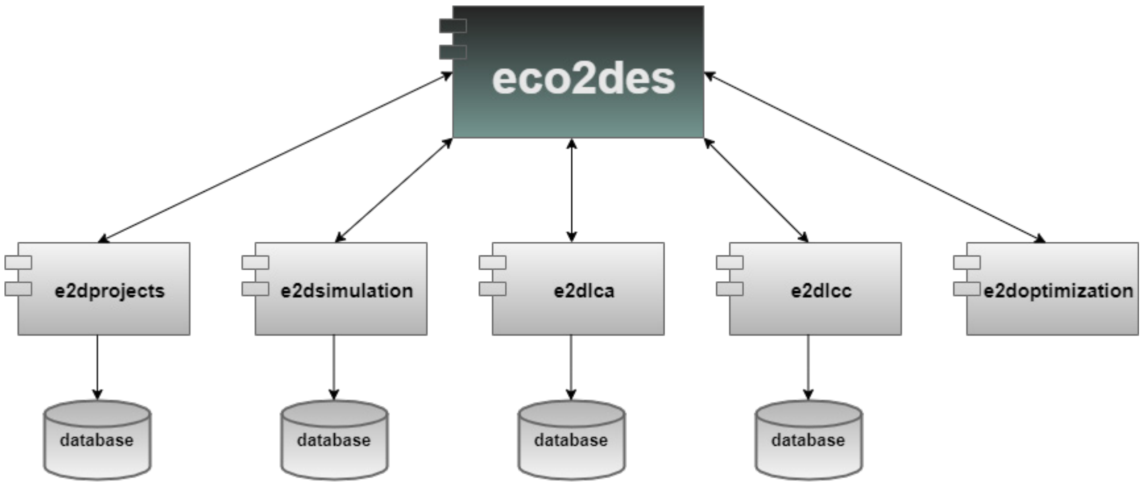

Figura 9. Arquitectura de eco2des

La herramienta eco2des es más que un simple conjunto de módulos; es una plataforma integrada que facilita la toma de decisiones informadas y sostenibles en la industria. Combina tecnología avanzada con un enfoque ambiental y económico, permitiendo a los profesionales enfrentar los desafíos de la sostenibilidad con herramientas de vanguardia. Con su enfoque sistemático y su sólida base en principios de ecodiseño, eco2des se posiciona como un activo valioso para cualquier organización que busque mejorar la eficiencia de sus procesos industriales mientras minimiza su impacto ambiental.

7. Casos de estudio

El marco metodológico y la herramienta propuestos para el ecodiseño de procesos industriales se validan mediante dos casos prácticos, expuestos en esta tesis. El primero se refiere a la metanación de dióxido de carbono para el almacenamiento de energía eólica en la red de gas natural. Este estudio se utiliza para demostrar las características clave de la herramienta eco2des y proporcionar orientación sobre su aplicación. El segundo caso de estudio trata la producción de combustibles sintéticos a partir de biomasa. Este complejo proyecto muestra la capacidad de eco2des para proporcionar diseños sostenibles y conclusiones fiables sobre tecnologías novedosas, como las que se están investigando para descarbonizar el sector industrial.

7.1. Metanación de CO_2 para el almacenamiento de energía eólica en la red de gas natural

7.1.1. Definición del objetivo y del alcance

Este caso de estudio utiliza la herramienta eco2des en la optimización de la sostenibilidad del proceso de producción de gas natural sintético (GNS) mediante la metanación de CO_2, donde se persigue la minimización simultánea de impactos ambientales y costes económicos. La configuración del sistema evaluado, que se puede visualizar en la Figura 10, abarca desde la captación de dióxido de carbono de una emisión industrial, pasando por la generación de hidrógeno vía electrólisis impulsada por electricidad eólica sobrante, hasta la síntesis y almacenaje estacional del GNS.

El enfoque del análisis se delimita desde la extracción de materias primas hasta la salida de la fábrica (cuna a puerta), enfocándose en la optimización de los parámetros de diseño del proceso. La unidad funcional del sistema se define como un metro cúbico en condiciones normales (Nm^3) de GNS producido. Para el estudio ambiental se ha seleccionado la base de datos ecoinvent 3.6 (Wernet et al. 2016), aplicando el modelo Cut-Off como sistema de fondo, y se ha elegido la categoría de calentamiento global para medir el impacto ambiental del proceso. En el aspecto económico, el rendimiento se mide a través del coste nivelado de producto (LCOP, por sus siglas en inglés, levelized cost of product) de GNS, cuantificado en euros por metro cúbico normal (€/Nm^3).

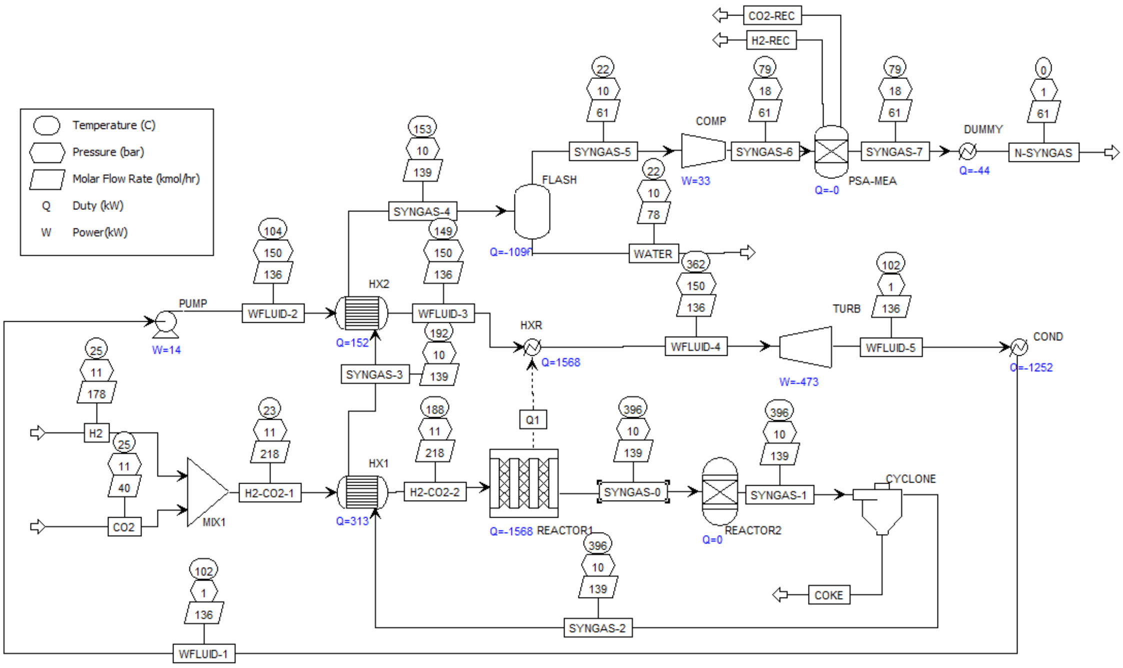

Figura 10. Diagrama de flujo en Aspen Plus del sistema de primer plano

7.1.2. Análisis del inventario predictivo del ciclo de vida (IPCV)

La generación del inventario predictivo inicia con la creación de la simulación del proceso (Figura 10) empleando el modelo cinético 12 de Kopyscinski (2010) y el enfoque de Langmuir-Hinshelwood para describir los mecanismos de reacción en dos etapas: la reacción de desplazamiento agua-gas y la formación de metano.

Tras completar la simulación, eco2des facilita la elaboración de un inventario ambiental predictivo vinculando las actividades del modelo de ACV con los resultados obtenidos de la simulación en Aspen Plus. Por ejemplo, la Figura 11 ilustra el procedimiento para crear un nuevo sistema de producto, mientras que la Figura 12 demuestra la adición de una corriente cuyos valores proceden directamente de la simulación.

```
e2d.project.lca.create_activity(
    name="Sabatier for renewable energy storage",
    location="ES",
    unit="normal cubic meter",
    ref_product="SNG",
    production_amount=1.0,
)

sabatier = e2d.project.lca.activities["Sabatier for renewable energy storage"]
```

Figura 11. Creación el sistema de producto en eco2des

```
def lci_wind_energy():

    hydrogen_in = e2d.project.simulation.streams["H2"]
    hydrogen_in_mass_flow, _ = hydrogen_in.output.total_mass_flow()
    hydrogen_rec = e2d.project.simulation.streams["H2-REC"]
    hydrogen_rec_mass_flow, _ = hydrogen_rec.output.total_mass_flow()
    hydrogen_mass_flow = hydrogen_in_mass_flow - hydrogen_rec_mass_flow

    electricity, _ = e2d.project.simulation.utilities["ELECTRICITY"].total_value

    sng = e2d.project.simulation.streams["N-SYNGAS"]
    sng_volume_flow, _ = sng.output.total_volume_flow()

    return (49 * hydrogen_mass_flow + electricity) / sng_volume_flow


wind_energy = [
    act
    for act in ei36
    if act["name"] == "electricity production, wind, >3MW turbine, onshore"
    and act["location"] == "ES"
][0]

sabatier.new_exchange(amount=lci_wind_energy, input=wind_energy, type="technosphere")
sabatier.save()
```

Figura 12. Añadir un input al sistema de producto conectado a la simulación en eco2des

Del mismo modo, para la creación del inventario del ACCV, eco2des calcula el CAPEX utilizando el método factorial descrito por Towler y Sinnott (2013a) para los componentes principales de la planta. Como ilustra la Figura 13, se extraen datos necesarios de la simulación para integrar el coste de un recipiente dentro del inventario económico en eco2des.

```python
def lcc_sabatier_flow():
    stream_in = e2d.project.simulation.streams["H2-CO2-2"]
    vol_flow, _ = stream_in.output.total_volume_flow()
    return vol_flow


def lcc_sabatier_rt():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    residence_time, _ = rplug.output.residence_time()
    return residence_time


def lcc_sabatier_ld():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    length, _ = rplug.output.length()
    diameter, _ = rplug.output.diameter()
    return length / diameter


def lcc_sabatier_pres():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    pressure, _ = rplug.output.pressure_max()
    return pressure


def lcc_sabatier_temp():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    temperature, _ = rplug.output.temperature_max()
    return temperature


capex.add_vessel(
    name="Methanation reactor",
    volume_flow=lcc_sabatier_flow,
    residence_time=lcc_sabatier_rt,
    length_diameter_ratio=lcc_sabatier_ld,
    pressure=lcc_sabatier_pres,
    temperature=lcc_sabatier_temp,
    vessel_kind="horizontal",
    material="Stainless 304",
    process_type="Fluids",
)
```

Figura 13. Añadir equipo al modelo de ACCV mediante una correlación de eco2des

La estimación del OPEX sigue una metodología análoga, donde la Figura 14 exhibe el proceso de instanciación de un objeto `opex` que sirve para incorporar diversos costes al inventario, tales como los salarios de los operadores (línea 3), financiación mediante préstamos (línea 7), depreciación de activos (línea 9), y costes de materias primas (líneas 12 a 27).

```
1  opex = e2d.project.lcc.opex
2
3  opex.operating_labour(
4      positions=4, employees=4.8, salary=30000, interannual_variance=0.015
5  )
6
7  opex.loan(percent=0.6, interest=0.04, years=10)
8
9  opex.depreciation(type="linear", value=0.07, residual_value=0)
10
11
12 def lcc_co2():
13
14     co2_in = e2d.project.simulation.streams["CO2"]
15     co2_in_mass_flow, _ = co2_in.output.total_mass_flow()
16     co2_rec = e2d.project.simulation.streams["CO2-REC"]
17     co2_rec_mass_flow, _ = co2_rec.output.total_mass_flow()
18     co2_mass_flow = co2_in_mass_flow - co2_rec_mass_flow
19
20     f = e2d.project.capacity_factor()
21
22     return co2_mass_flow / 1000 * f * 8760
23
24
25 opex.add_raw_material(
26     name="CO2", quantity=lcc_co2, price=10, interannual_variance=0.015, unit="Tn"
27 )
28
```

Figura 14. Cálculo del OPEX en eco2des

7.1.3. Evaluación del impacto del ciclo de vida (EICV)

En la evaluación del impacto del ciclo de vida, el indicador seleccionado para valorar el rendimiento ambiental fue el potencial de calentamiento global, utilizando el método del Panel Intergubernamental sobre Cambio Climático (IPCC) del año 2013 (Stocker et al. 2013), y dejando de lado las emisiones a largo plazo. En paralelo, para medir el rendimiento económico, se estableció el coste nivelado de producción (LCOP) de GNS. Se empleó una tasa de descuento, en base a la rentabilidad esperada, del 10% para el cálculo del LCOP, presuponiendo una duración operativa de la planta de 30 años y un lapso de construcción de 1,5 años.

7.1.4. Optimización multiobjetivo

El estudio se articula en dos problemas de optimización distintos. El primero es tridimensional y busca la minimización tanto del impacto de calentamiento global como del LCOP, además de maximizar la eficiencia del sistema de almacenamiento, calculada como el valor calorífico inferior del GNS dividido por la energía eléctrica utilizada en su producción. Una evaluación preliminar revela que los objetivos ambientales y económicos no se contraponen, lo cual conduce a la formulación de un segundo problema de optimización bidimensional, que se centra en la minimización del LCOP y la maximización de la eficiencia de almacenamiento.

Para abordar eficientemente estos problemas de optimización multiobjetivo y hallar soluciones adecuadas, se recurre a la implementación de algoritmos genéticos en eco2des. El algoritmo evolutivo multiobjetivo con descomposición (MOEA/D) propuesto por Zhang y Li en 2007 se utilizó para el primer problema, mientras que para el segundo se optó por el algoritmo genético de clasificación no dominada II (NSGA-II) desarrollado por K. Deb et al. en 2002. Las restricciones pertinentes se manejaron a través del método de penalización por muerte, descrito por Back en 1991.

La Figura 15 ejemplifica el modo en que se define el problema de optimización en eco2des, previa especificación de las funciones objetivo, las variables de decisión y las restricciones.

```python
algorithm = e2d.optimization.moead(gen=20)

problem = e2d.project.optimization.problem(
    variables=(
        h2_co2_ratio,
        reactor_temp,
        reactor_length,
        reactor_ld_ratio,
        working_fluid,
    ),
    bounds=([4, 250, 1, 1, 0], [5, 400, 20, 10, 1]),
    objectives=(gw, lcop, eff_storage),
)

initial_population = e2d.project.optimization.population(problem, 190)

evolved_population = algorithm.evolve(initial_population)

```

Figura 15. Definición del problema de optimización y resolución del mismo en eco2des

7.1.5. Interpretación

El análisis de los datos obtenidos revela la viabilidad de alcanzar un rendimiento ambiental y económico no conflictivo en la metanación de CO_2 para el almacenamiento de energía eólica en la red de gas natural. Además, del estudio realizado sobre la eficiencia de almacenamiento como objetivo potencialmente conflictivo, se deduce que los incrementos en eficiencia no compensan el aumento de costes e impactos ambientales, tal como muestra la Figura 16. Por ende, se opta por resolver el problema centrándose en un objetivo único: la minimización del impacto ambiental junto al coste. De este modo se identifican las condiciones operativas óptimas y las decisiones de diseño de proceso más acertadas. Este escenario se caracteriza por un LCOP de 1,48 €/Nm^3, un impacto de 1,09 kg CO_2-eq./Nm^3 y una eficiencia de almacenamiento del 57,95%, bajo las siguientes condiciones específicas: una relación H_2/CO_2 de 4,44, una temperatura en el reactor de 396°C, una longitud de reactor de 2,64 m, una relación longitud-diámetro de 5,72 y el empleo de agua como fluido de trabajo en los recuperadores de calor que alimentan un ciclo de Rankine.

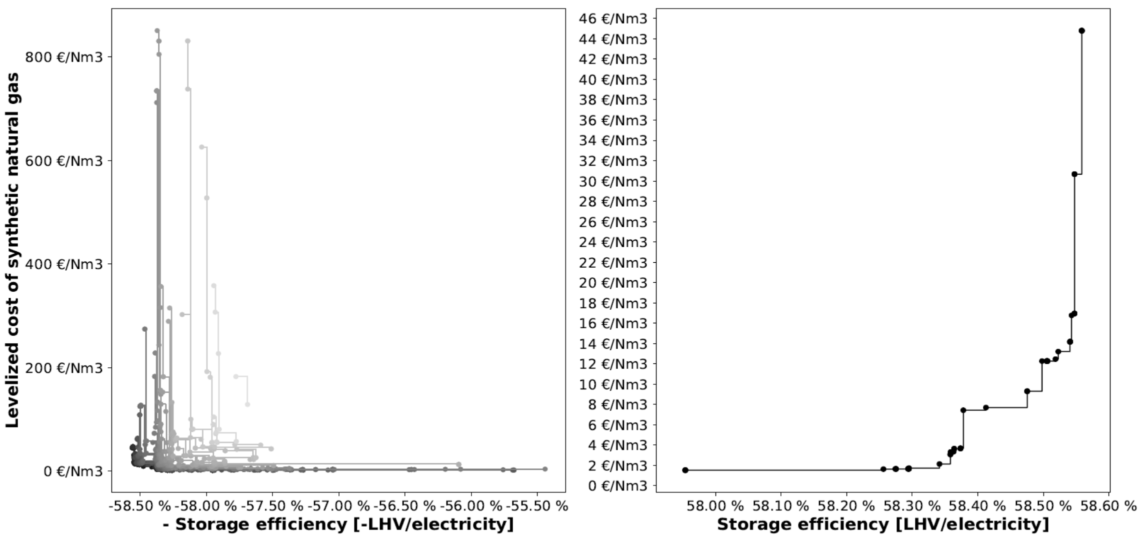

Figura 16. Resultados de la optimización para el problema 2, LCOP vs eficiencia de almacenamiento

7.2. Producción de biocombustibles

7.2.1. Definición del objetivo y del alcance

El propósito de este estudio consiste en optimizar tanto el rendimiento económico como el ambiental en una refinería dedicada a la coproducción de biocombustibles sintéticos y electricidad a partir de biomasa. Este objetivo se aborda desde una perspectiva integral de ciclo de vida. El sistema en primer plano se detalla en la Figura 17, abarcando desde el suministro de biomasa y materias primas, pasando por el aporte energético al proceso, hasta llegar a la producción efectiva de biocombustibles. La revisión bibliográfica indica que una planta con una capacidad de procesamiento de 2.000 toneladas diarias de biomasa se considera viable económicamente (Hamelinck et al. 2004; Leibbrandt et al. 2013; Rafati et al. 2017). Fundamentado en estos estudios previos, la planta de nuestro análisis parte de procesar esta cantidad estipulada, incrementándola a 2.800 toneladas por día en la etapa de interpretación del ciclo de vida.

El análisis del ciclo de vida (ACV) se realiza empleando la base de datos ecoinvent versión 3.6 (Wernet et al. 2016), bajo el modelo Cut-Off. Por su parte, el análisis de costes del ciclo de vida (ACCV) se lleva a cabo utilizando el método del valor presente neto para el cálculo del capital de inversión (CAPEX) y los costes operativos (OPEX) a lo largo del ciclo de vida completo de la biorrefinería, dejando fuera las externalidades.

El estudio establece un enfoque de cuna a puerta para delimitar el sistema de producto, criterio que se considera idóneo para optimizar los parámetros de diseño y operación del proceso. La unidad funcional definida para el sistema es 1 kWh de combustibles (comprendiendo hidrógeno, gasolina, queroseno y diésel), basada en el poder calorífico inferior de los mismos. Las categorías de impacto ambiental que se evalúan en profundidad son el calentamiento global y el agotamiento de los recursos fósiles. Paralelamente, el valor actual neto (VAN) se establece como la métrica de referencia para evaluar el rendimiento económico del sistema.

7.2.2. Análisis del inventario predictivo del ciclo de vida (IPCV)

En la estructura de la biorrefinería contemplada para este estudio, se consideran únicamente tecnologías que ya están disponibles comercialmente, lo que posibilita su implementación inmediata en el proceso de gasificación de biomasa acoplado al procesamiento Fischer-Tropsch (FT). La Figura 17 ilustra de forma esquemática los principales pasos involucrados en la producción de combustibles y electricidad, destacando las siguientes unidades: ASU (unidad de separación de aire, *air separation unit*), WGS (reactor de desplazamiento agua-gas, *water gas shift*), AGR (eliminación de gases ácidos, *acid gas removal*), FT (síntesis Fischer-Tropsch), PSA (unidad de adsorción por cambio de presión, *pressure swing adsorption*), ATR (reactor de reformado autotérmico, *autothermal reforming*), CHP (planta de generación eléctrica, *combined heat and power*) y HC (unidad de hidrocracking).

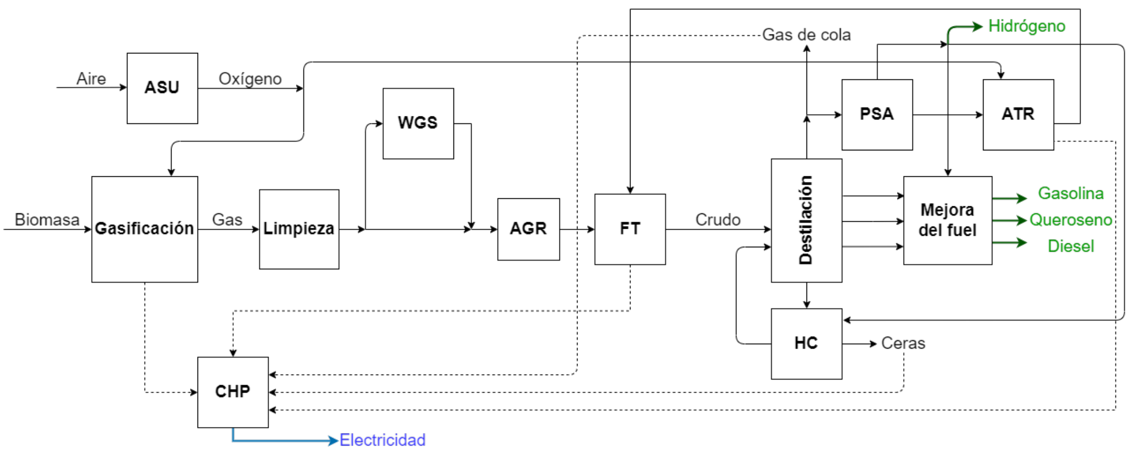

Figura 17. Diagrama de flujo de la biorrefinería. La línea discontinua representa flujos de calor.

El gas de síntesis obtenido de la gasificación puede derivarse de distintas materias primas tales como biomasa, carbón, coque de petróleo o residuos sólidos municipales. Este estudio se enfoca en la biomasa, específicamente el maíz, pero el modelo está diseñado para adaptarse a cualquier tipo de sólido basado en carbono, siempre y cuando su composición se defina a través de un análisis último y próximo. El gas de síntesis necesita un tratamiento adicional para la eliminación de contaminantes e impurezas. Además, para el proceso FT es esencial ajustar la relación H_2/CO y reducir el contenido de CO_2. Una vez limpio y acondicionado, el gas de síntesis se convierte en hidrocarburos mediante un reactor de síntesis FT. Los productos resultantes de este proceso se separan y se convierten en distintos combustibles líquidos mediante operaciones comparables a las empleadas en refinerías de petróleo convencionales (Steynberg y Nel 2004). Los gases residuales de la destilación se canalizan hacia una unidad PSA, donde se recupera hidrógeno para ser utilizado en la mejora de combustibles, equilibrando la relación H_2/CO del gas de síntesis y como producto final. Posteriormente, un ATR transforma los hidrocarburos ligeros en más gas de síntesis que se reincorpora al ciclo. Además, las ceras obtenidas en la destilación se someten a un proceso de craqueo para su reintroducción en el sistema de destilación. La configuración de este proceso integrado se modela en Aspen Plus utilizando la ecuación de estado de Soave-Redlich-Kwong (SRK) para todas las corrientes, excepto para las de agua pura, que se modelan usando las tablas de vapor de NBS/NRC.

Con la simulación completada, se emplea eco2des para construir el inventario predictivo que vincula los resultados de la simulación con los modelos de análisis del ciclo de vida (ACV) y análisis de costes del ciclo de vida (ACCV).

7.2.3. Evaluación del impacto del ciclo de vida (EICV)

Una vez implementado el inventario predictivo del ciclo de vida de la biorrefinería en eco2des, se evalúan dos categorías de impacto ambiental: el calentamiento global y el agotamiento de recursos fósiles. La primera se calculó utilizando los potenciales de calentamiento global del método IPCC 2013 (Stocker et al. 2013) sin emisiones a largo plazo, y la segunda se calculó utilizando el método ReCiPe Midpoint (H) v1.13 (Huijbregts et al. 2016). Por su parte, para la evaluación del impacto económico, se calcula el VAN con una tasa de interés nominal del 5%, siguiendo las recomendaciones expuestas en las normas ISO de la serie ACCV para la industria del petróleo y el gas natural (ISO 2021).

7.2.4. Optimización multiobjetivo

En este estudio se proponen dos problemas de optimización multiobjetivo (MOOP, por sus siglas en inglés) para minimizar el potencial de calentamiento global (GWP, también en inglés) y maximizar el Valor Actual Neto (VAN). El primer problema (MOOP1) se orienta hacia la consecución de estos objetivos específicos, mientras que el segundo (MOOP2) incluye, adicionalmente, la maximización de la producción de queroseno. Ambos MOOPs comparten cinco variables de decisión, que se presentan en la Tabla 1, con rangos establecidos tras un análisis de sensibilidad preliminar realizado con la herramienta eco2des.

Tabla 1. Problemas de optimización multiobjetivo para la producción de biocombustibles

Funciones objetivo		
MOOP1	$Min(GW, -VAN)$	
MOOP2	$Min(GW, -VAN, -Queroseno)$	
Variables de decisión	**Límite inferior**	**Límite superior**
Temperatura de gasificación	700 °C	900 °C
Ratio vapor/biomasa	0	1,5
Temperatura de FT	200 °C	250 °C
Velocidad espacial horaria de gas (GHSV)	1000 $cm^3/h/g_{cat}$	6000 $cm^3/h/g_{cat}$
Ratio H_2/CO	1,5	2,5

El MOOP1 se abordó utilizando el algoritmo genético de ordenación no dominada II (NSGA-II) (K. Deb et al. 2002), mientras que para el MOOP2 se empleó el algoritmo evolutivo multiobjetivo con descomposición (MOEA/D) (Zhang y Li 2007).

7.2.5. Interpretación

La optimización realizada en el MOOP1 expone una frontera de Pareto con una forma sigmoidal característica (ilustrada en la Figura 18), donde se observa la presencia de metas en conflicto con valores positivos y negativos de la huella de carbono del proceso, determinados principalmente por la producción de electricidad en la planta. Por otro lado, se obtiene un VAN más elevado al reducir la producción excedente de electricidad, lo que conlleva a una conversión más eficiente de la biomasa en combustibles. En cuanto a las variables de decisión, la temperatura de gasificación, la relación vapor-biomasa y el GHSV ejercen una influencia notable en la eficacia de la biorrefinería. Las altas temperaturas de gasificación favorecen la disminución del impacto en el cambio climático, mientras que las más bajas potencian la conversión de biomasa en combustibles. La proporción vapor-biomasa óptima se encuentra entre 0,67 y 1,19, con un VAN superior para valores por debajo de 0,9. Los valores de GHSV cercanos al límite inferior de su espacio de decisión reducen el impacto climático y aquellos más elevados mejoran el VAN mediante un incremento en la producción de hidrógeno. El intervalo de la relación H_2/CO fluctúa entre 2,22 y 2,49, con valores superiores al estequiométrico que benefician el rendimiento económico al incrementar la producción de hidrógeno.

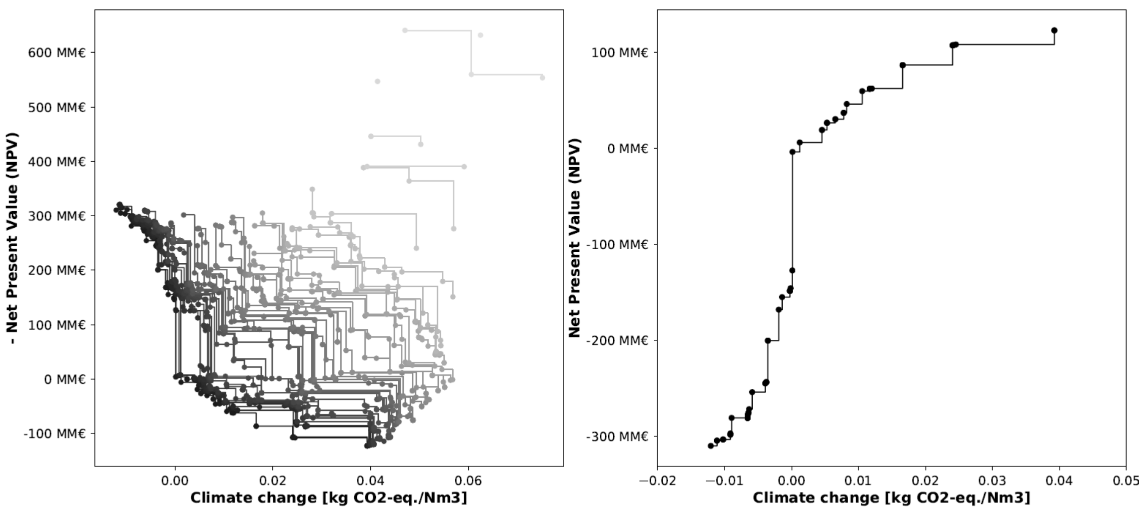

Figura 18. Resultados del MOOP1 en eco2des, VAN vs cambio climático

Por otra parte, la optimización del MOOP2 demuestra que la inclusión del objetivo de maximizar la producción de queroseno introduce nuevos conflictos (Figura 19). La producción de queroseno está fuertemente influenciada por el GHSV, donde valores inferiores maximizan su producción, pero reducen la eficiencia económica de la biorrefinería debido al mayor consumo de hidrógeno necesario para el hidrocracking de las ceras. La relación de vapor a biomasa y la relación H_2/CO impactan en menor medida la producción de queroseno. Sin embargo, la relación óptima vapor-biomasa para maximizar la producción de queroseno se sitúa entre 0,1 y 0,6, y una relación H_2/CO cercana al valor estequiométrico de 2 favorece la maximización de este combustible.

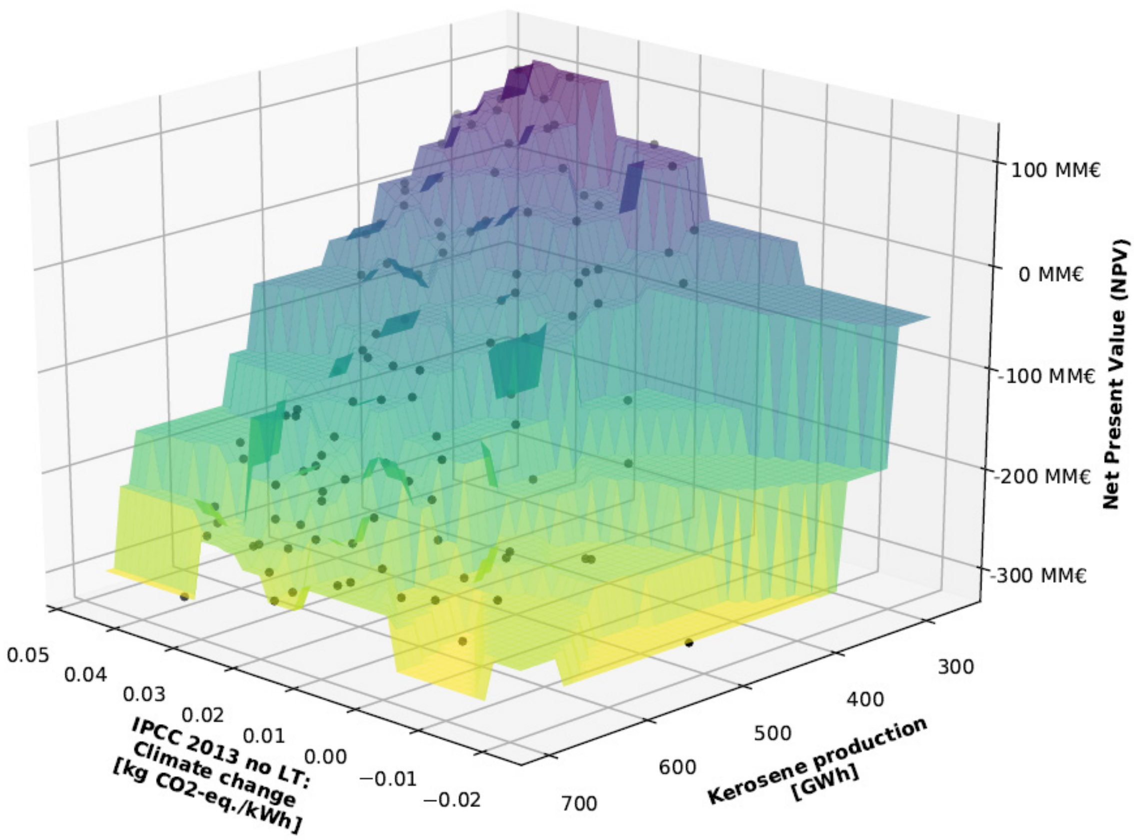

Figura 19. Resultados del MOOP2 en eco2des, VAN vs cambio climático vs producción de queroseno

Además, se ha desarrollado un caso tomando parámetros de referencias literarias (Rafati et al. 2017; Leibbrandt et al. 2013; Dry 2002; Visconti and Mascellaro 2013; Méndez and Ancheyta 2020), y se han establecido cuatro escenarios basados en los resultados de los MOOPs: el escenario 1 maximiza el VAN, el escenario 2 minimiza el GWP manteniendo el VAN en un umbral no negativo, el escenario 3 maximiza la producción de queroseno con la misma restricción de VAN, y el escenario 4 representa una condición intermedia en la que el VAN es del torno de los 50 M€ minimizando impactos ambientales y con la máxima producción de queroseno posible. Los resultados, presentados en la Tabla 2, sugieren que la coproducción de hidrógeno y combustibles líquidos puede ser una estrategia viable para mejorar el desempeño económico y ambiental, a pesar de que podría implicar una disminución en la producción de queroseno.

Tabla 2. Caso de referencia vs escenarios óptimos

		Referencia	Escenario 1	Escenario 2	Escenario 3	Escenario 4
Variables de decisión	T gasificación, °C	827,00	716,59	882,20	734,86	827,06
	Vapor / biomasa (w/w)	0,35	0,67	1,19	0,46	1,05
	FT T, °C	220,00	248,48	222,88	248,42	203,62
	FT GHSV, $cm^3/h/g_{cat}$	3600,00	5973,96	5473,92	4398,44	5217,37
	H_2/CO ratio (mol/mol)	2,15	2,49	2,43	2,18	2,49
Producción de energía, kWh	Hidrógeno	850,26	1367,75	1183,26	1060,02	1197,74
	Gasolina	555,83	348,23	324,45	473,74	361,73
	Queroseno	452,1	298,97	272,99	396,53	302,22
	Diesel	242,94	154,92	142,3	210,15	158,1
	Electricidad	-27,96	17,58	198,59	-5,73	138,79
	Rendimiento energético	47,96%	50,60%	49,08%	49,38%	49,93%
Impactos de sostenibilidad	VAN, M€	-98,71	122,7	5,81	3,92	49,34
	GW, kg CO2-eq. / kWh	0,049	0,039	0,001	0,044	0,015
	FD, kg oil-eq. / kWh	0,016	0,012	-0,011	0,014	-0,003

Las conclusiones más relevantes obtenidas de la optimización indican que: (i) la naturaleza y cantidad de subproductos generados por la biorrefinería influyen considerablemente en su rendimiento, siendo el precio de mercado de los mismos un actor determinante; (ii) hay una tendencia a reducir la producción de queroseno en los procesos de optimización, probablemente debido a su menor valor de mercado en comparación con el hidrógeno; y (iii) la integración de un modelo de simulación de procesos junto con inventarios de ACV y ACCV facilita la configuración de escenarios sostenibles, gracias a la generación de soluciones óptimas a través de algoritmos genéticos.

Estos hallazgos subrayan la complejidad de balancear las metas de sostenibilidad ambiental con las económicas en el diseño y operación de biorrefinerías. La capacidad de los modelos de simulación y los métodos de optimización para predecir y reconciliar estos conflictos es crucial para el desarrollo de tecnologías de energía renovable que sean tanto económicamente viables como ambientalmente responsables. El estudio amplía la comprensión de cómo las decisiones operativas y de diseño pueden influir en la huella ambiental y la rentabilidad, ofreciendo una herramienta valiosa para los responsables de la toma de decisiones en la industria de la bioenergía.

8. Discusiones y conclusiones generales

La presente investigación ha culminado en el desarrollo y validación de un novedoso marco metodológico de ecodiseño para la ingeniería de procesos industriales, probando su eficacia en la generación de escenarios óptimos que se alinean con los criterios de sostenibilidad. La herramienta eco2des, una pieza central de esta tesis, se ha revelado como un sistema de apoyo a la decisión robusto y versátil en dos casos de estudio distintos, reafirmando su valor para la realización de análisis de ecodiseño holísticos y para el impulso en la reducción de tiempos hacia la comercialización de nuevos procesos industriales sostenibles.

En el estudio específico de la metanación, la utilidad de eco2des se ha manifestado en la ejecución de un estudio de ecodiseño mediante una implementación en Python, evidenciando el equilibrio entre el alcance analítico del software y la simplicidad en su uso. El segundo caso, enfocado en la biorrefinería, ha servido para demostrar que el diseño de procesos bajo enfoques tradicionales puede resultar subóptimo cuando se evalúa bajo la lente de la sostenibilidad. Esto subraya la necesidad imperante de una metodología integrada como la propuesta en este trabajo para el diseño de procesos industriales. Se debe enfatizar la relevancia de los modelos predictivos y rigurosos en el contexto de eco2des, que aseguran la precisión de los resultados obtenidos. Si el modelo que alimenta el inventario predictivo del ciclo de vida no es robusto, los resultados obtenidos no serán fiables.

Durante el desarrollo de eco2des, se identificó como desafío principal la ausencia de una interfaz de datos estandarizada, lo que dificultó la interoperabilidad entre sistemas. La digitalización y estandarización emergen, por lo tanto, como habilitadores esenciales para alcanzar la interoperabilidad de herramientas que impulsan soluciones sostenibles.

Mirando hacia el futuro, se plantea la necesidad de integrar el análisis social del ciclo de vida (ASCV) dentro de la metodología, para capturar todas las facetas de la sostenibilidad. Asimismo, es esencial avanzar en el desarrollo de soluciones digitales que operen en tiempo real, beneficiándose de la recolección instantánea de datos para optimizar la toma de decisiones y la eficiencia procesal, lo cual permitiría ajustes dinámicos en los sistemas en estudio y mejoras continuas. En este horizonte, la investigación futura debería explorar el potencial de los modelos predictivos impulsados por inteligencia artificial (IA), en concreto, redes neuronales, para la creación del inventario predictivo del ciclo de vida. Esto facilitaría una optimización aún más efectiva y una toma de decisiones en tiempo real, aplicando la metodología y la herramienta desarrolladas en la presente tesis, no solo al diseño, sino que también a la operación de procesos.

En suma, este trabajo sienta las bases para un avance significativo en la integración de criterios de sostenibilidad en el diseño de procesos industriales, con el potencial de transformar los paradigmas de producción hacia modelos más respetuosos con el medio ambiente sin dejar de lado la viabilidad técnica y el rendimiento económico de los mismos.

EXECUTIVE SUMMARY

1. Motivation

The motivation for this research stems from the increasing concern within companies, governments, and consumers regarding sustainable production and consumption. In this behalf, the concept of life cycle thinking (LCT) has become central to promoting sustainability and integrating it into all aspects of product development and consumption. Furthermore, several policies have emerged to promote sustainability. The EU has been a leader in applying LCT to policy development, and its policies have served as examples for other regions. The industry sector is crucial to achieving sustainability, as it accounts for a significant proportion of greenhouse gas emissions, biodiversity loss, and water stress. The challenge lies in incorporating and standardizing the concept of sustainability across different sectors, especially in the industrial sector, which plays a critical role in promoting progress and prosperity. Therefore, this thesis aims to develop a unique methodology, integrated in a tool, that combines process simulation, life cycle analysis (LCA), and life cycle costing (LCC) methodologies for their holistic application in the economic and environmental optimization of any industrial process under research and/or development.

2. Objectives

The goal of this thesis is to define an eco-design methodology for sustainability-based optimization of industrial processes by combining process simulation, LCA, LCC, and mathematical optimization. Furthermore, the methodology will be encapsulated in a computer-based software for future application. To achieve this goal several objectives are identified in the research plan:

- Reviewing the state-of-the-art of applications, methodologies and frameworks that combines predictive and descriptive models with LCA, LCC and multiple-criteria decision analysis.
- Stablishing a holistic methodology for the sustainability-based optimization of industrial processes based on process simulation, LCA, LCC and mathematical optimization.

- Developing a precommercial software for the computer aided sustainability-based optimization of industrial processes based on the formulated methodology.
- Testing and validating the methodology and software.

3. State-of-the-art review

Within this thesis the state-of-the-art review explores the integration of techno-economic analysis (TEA), in particular those that combine process simulation with life cycle costing (LCC); life cycle assessment (LCA), and multiple criteria decision analysis (MCDA) methodologies for the eco-design of industrial processes. The review highlights the potential benefits and versatility of this integrated approach across various industrial sectors, including biofuel production pathways, carbon dioxide revalorization, and water treatment. By examining these diverse applications, the review showcases the adaptability of TEA, LCA, and MCDA integration in driving sustainable-based decisions across a wide range of industries.

The state-of the-art review of applications reveals that an increasing number of practitioners are incorporating combined TEA-LCA to assess the environmental and economic aspects of implementing new technologies and to perform multi-objective optimization to optimize process pathways. However, despite the value of integrating LCA and LCC (including TEA) for sustainability assessments, there is a lack of consistency in criteria and methodology, leading to the absence of formal guidance for selecting a suitable integration procedure for diverse objectives. Therefore, also a review of frameworks that aim to integrate these methodologies is conducted, showing that some efforts have been done in this area. However, there is a lack of harmonization and none of them cover all the methodologies identified as key drivers for the eco-design framework for industrial processes that is developed within this thesis.

The review also identifies a growing interest in the prospective application of integrated TEA and LCA tools to assess emerging technologies at early technology readiness levels (TRLs). Nonetheless, most existing applications are focused on specific industries, lacking interoperability in the broader process engineering field.

In conclusion, an integrated methodology can significantly benefit technology developers in creating sustainable processes by allowing simultaneous evaluation of economic and environmental viability, as well as process optimization in terms of the lowest production cost and lowest environmental impacts. Further research is required to provide a consistent framework and tools that will benefit both technology developers and policymakers, ultimately promoting the adoption and development of an integrated approach for eco-design in industrial processes.

4. Materials and methods

4.1. Process simulation

Process simulation is conducted using a step-by-step approach: problem analysis, data input, execution, and results analysis. During the problem analysis, the actual process flow diagram is adapted to the software capabilities and simulation goals to create a process simulation diagram. This involves examining the chemistry, converting the process flow diagram, determining the appropriate thermodynamic model, and analyzing the degrees of freedom. Then, data input is carried out depending on the capabilities of the selected process simulation software, with input data collected from the problem analysis or predefined convergence options. Components, thermodynamic models, process flowsheets, input streams, and unit definitions are all considered. Convergence options include computational sequence, computation strategy, initial data for tear streams, and convergence criteria. Furthermore, the execution step involves running the simulation and obtaining results, such as stream reports, unit reports, unit performances, and physical properties. Finally, results analysis consists of validating the convergence and reliability of the results. If the simulation converges, users must verify mass and energy balances, revise recycle streams flow rates, and check product streams. If convergence issues arise, various troubleshooting steps can be taken to identify and resolve problems. Once reliability is ensured, additional analyses such as sensitivity analysis, case studies, and multi-variable optimization can be conducted to extract more value from the simulation results.

By integrating process simulation into the eco-design framework, inventory data for subsequent environmental and economic models can be directly extracted from the simulation results. The Aspen ONE engineering suite (AspenTech 2022b) is the leading process simulation software, offering an integrated system for computer-assisted process engineering, including flowsheeting systems and specialized packages. Within this suite, Aspen Plus is a steady-state simulation environment that includes a comprehensive database and several thermodynamic models, frequently used for process design and techno-economic analyses in various industries. Aspen Plus was chosen as the commercial software for the development of this thesis due to its wide range of applications in chemical, biofuel, and power plant engineering.

4.2. Life cycle assessment (LCA)

LCA is a standardized approach used to evaluate the environmental burdens of an industrial process. It follows international standards, ISO 14040 and 14044 (ISO 2006a; 2006b), and comprises four main steps: goal and scope definition, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA), and life cycle interpretation.

The goal and scope definition involves establishing the objective, functional unit, system boundaries, and other methodological aspects of the study. The LCI phase consists of collecting inventory data, addressing multifunctionality, and defining the allocation procedures. The LCIA phase aggregates environmental flows into impact categories, potentially including normalization and weighting steps, and selects the appropriate impact assessment method. Finally, the life cycle interpretation phase identifies significant issues, evaluates the completeness, sensitivity, and consistency of the study, and presents conclusions, limitations, and recommendations.

Through the incorporation of the LCA methodology into the eco-design framework, researchers can evaluate and improve the environmental performance of industrial processes throughout their entire life cycle. The market offers a variety of LCA software tools, ranging from commercial licenses to open-source frameworks. The selection of a tool depends on various factors, including functionality concerns, database availability, user interface, data quality and management, and modeling principles. For this thesis, Brightway2 (Mutel 2017), an open-source LCA framework, was selected due to its powerful features, availability of environmental databases, ease of integration into the eco-design tool being developed, fast calculations, and no identified lack of functionalities.

4.3. Life cycle costing (LCC)

The LCC methodology comprises several stages, including goal and scope definition, data collection, costs assessment, and interpretation. The goal and scope definition outlines the study's objectives, system boundaries, economic performance indicators, and data sources. Data collection involves gathering economic assessment data and identifying cost drivers such as net present value (NPV), internal rate of return (IRR), payback period or the levelized cost of production (LCOP). Costs assessment focuses on estimating capital expenditure (CAPEX), operating expenditure (OPEX), and generating a cash flow model to determine economic performance indicators. The CAPEX of an industrial process is the total cost of designing, constructing, and installing it. While the OPEX are the costs associated with production expenses that are incurred independently of the plant output or operation rate (fixed costs) and the costs that are proportional to the plant output or operation rate (variable costs), including: raw materials, utilities, consumables, effluent disposal and packaging and shipping. Lastly, the interpretation phase identifies significant issues, evaluates completeness, sensitivity, and consistency checks, and draws conclusions, limitations, and recommendations for the study. The LCC methodology, as any LCT approach, is iterative, improving data quality and accuracy throughout the study.

By integrating the conventional LCC methodology into the eco-design framework, researchers can evaluate and improve the economic performance of industrial processes in a cradle-to-gate approach. There are several cost estimation tools for process engineering, including commercial and widely used Excel spreadsheet-based tools. However, these tools have limitations such as lack of flexible cash flow modeling or difficulties in automation and integration. Therefore, a new cost estimation tool is developed for this thesis using Python (Python Software Foundation 2022).

4.4. Multi-objective optimization

In real-world scenarios, most optimization problems involve satisfying multiple conflicting objectives, making them multi-objective optimization problems (MOOPs). Solving MOOPs results in a Pareto optimal front, a set of solutions where each solution is not dominated by any other in terms of all objectives. With this information, decision-makers can then choose the best trade-off solution based on their preferences.

The multi-objective optimization approach involves several key steps. The first one is the problem analysis, which involves: understand the optimization objectives, define the decision space, identify the functions relating decision variables to objectives, perform sensitivity analysis, and identify problem constraints. Next step is the formulation of the multi-objective optimization problem. Then, the optimization algorithm must be chosen, selecting a suitable option for the problem. Meta-heuristic algorithms are preferred as they perform better in complex and broad problems. Finally, in the results analysis step the Pareto front decision vectors are evaluated to understand the decision space and fine-tune variables that impact the optimal points. To analyze the performance of the chosen algorithms and to select the best one based on metrics like generational distance, spread, and hypervolume indicator are also carried out within this phase.

This is an iterative process that helps in reaching a reliable solution, which can be further analyzed using qualitative methods and visualization techniques. Stakeholders can then select a trade-off solution for in-depth analysis and understanding the problem's characteristics.

Through the incorporation of multi-objective optimization into the eco-design framework, stakeholders can evaluate several optimal scenarios that are produced automatically. The selected optimization library for this thesis is pygmo (Biscani and Izzo 2020), which is a scientific Python library for massively parallel optimization. It was chosen because of its unified interface to optimization algorithms and problems, wide range of optimization algorithms, and object-oriented design, which makes it easy to create custom classes and its integration within the eco-design tool.

5. Eco-design framework for industrial processes

One main objective of this thesis is to produce an eco-design framework for industrial processes. Since the growing demand for sustainable production and consumption has led to the need for an integrated and interoperable methodology that combines environmental impact assessments and cost analyses for the industrial sector. The eco-design framework for industrial processes aims to unify existing standards and methods while addressing challenges in comparing environmental impacts and costs, maintaining consistent data sources, and reducing trial-and-error phases during technology upscaling.

The framework is based on life cycle thinking methodologies, process simulation, and multi-objective optimization to develop an integrated methodology for the eco-design of industrial processes. The approach consists of several stages, including goal and scope definition, predictive life cycle inventory analysis (P-LCI), life cycle impact assessment (LCIA), multi-objective optimization, and life cycle interpretation.

During the goal and scope phase the objective, scope, and intended application are defined. This includes describing the product system, functional unit, system boundaries, allocation procedures, LCIA methodology, LCC performance indicators, optimization objectives, decision space, problem constraints, interpretation, data requirements, assumptions, limitations, data quality requirements, and the format of the report.

The P-LCI phase defines the coordinated procedure for collecting inventory data for the LCA and LCC models. This iterative process leads to a parametrized and predictive inventory connected to the simulated process, enabling automatic adjustments within the inventory in response to input modifications in the simulation. Therefore, the process simulation model is created iteratively to provide the necessary inputs for the LCA and LCC models while ensuring convergence in the decision space for the optimization problem, acting as a source of inventory data.

The next step is the LCIA, in which the predictive inventory data collected during the P-LCI phase is used by the LCA and LCC models to compute environmental and economic impacts. While during the multi-objective optimization phase, the optimization problem is formulated in synchrony with the predictive life cycle inventory and life cycle impact assessment phases, defining objectives, decision space, and technical constraints.

Finally, the interpretation phase includes identifying significant issues, evaluating the completeness, sensitivity, and consistency of the study, and providing conclusions, limitations, and recommendations for the intended audience. The inclusion of multi-objective optimization (MOO) in the eco-design framework allows for easier interpretation of results and insights into the main hotspots of the system and its sustainability performance under different process conditions.

6. Eco-design tool for industrial processes: eco2des

Together with the framework, the development of a holistic and integrated tool that encapsulates it is one of the key objectives of this thesis. The eco-design tool for industrial processes, eco2des, is a comprehensive framework aimed at facilitating environmentally conscious and economically viable design decisions for industrial processes. Combining process simulation, life cycle assessment (LCA), life cycle costing (LCC), and optimization techniques, eco2des enables users to evaluate the environmental impact, economic performance, and trade-offs of various process alternatives.

The eco2des framework comprises five core modules: e2dprojects, e2dsimulation, e2dlca, e2dlcc, and e2doptimization.

1. **e2dprojects**: This module enables users to manage project-related tasks, including creating, deleting, renaming, and copying projects. A project encapsulates a unique process simulation and its relations with its LCA model, LCC model, and optimization problem. Projects are stored in an SQLite database and as directories in the filesystem, allowing for efficient data organization and management.

2. **e2dsimulation**: This module allows users interacting with the simulation file linked to the project, enabling modification of simulation inputs, running the

simulation, and reading results. The module connects to Windows programs using the Component Object Model (COM), supporting various simulation entities and enabling seamless interaction with programs such as Aspen Plus. The e2dsimulation module provides a flexible structure for future integration with other computer-aided process engineering tools.

3. **e2dlca**: The e2dlca module assesses the environmental impacts of industrial processes using a matrix-based life cycle assessment (LCA) approach, inheriting most of its capabilities from the open-source Brightway2 framework. To improve performance, e2dlca caches matrices in memory, reducing the time spent on I/O operations, including capabilities to directly interact with matrices values. This optimization is crucial for evaluating thousands of scenarios in multi-objective optimization problems. The module also offers postprocessing functionalities for life cycle interpretation, such as visualizing top contributors and generating interactive Sankey diagrams.

4. **e2dlcc**: This module assesses the life cycle costing (LCC) of industrial processes, providing a comprehensive understanding of the economic aspects of the process, including capital expenditure (CAPEX) and operational expenditure (OPEX). The module also offers a cash-flow model for industrial processes and supports the life cycle interpretation phase for economic data with plots to enhance data visualization.

5. **e2doptimization**: This module is responsible for solving optimization problems, allowing users to define decision variables, constraints, and objectives from the process simulation, the LCA model, and/or the LCC model. It offers several algorithms for heuristic global optimization with single or multiple objectives. The module provides functionalities to support the life cycle interpretation phase, including plotting the Pareto front and exporting optimization results to Excel.

The eco2des tool offers a holistic approach to eco-design, enabling users to make well-informed decisions for sustainable industrial process development. By integrating project management, simulation interaction, environmental impact assessment, economic evaluation, and optimization techniques, eco2des provides a valuable tool for industries striving to minimize their environmental footprint while maintaining profitability and competitiveness.

7. Case studies

The proposed methodological framework and tool for the eco-design of industrial processes is validated through two case studies. The first case study relates to the carbon dioxide methanation for wind energy storage in the natural gas grid. This study is used to demonstrate the key features of the eco2des tool and provide guidance on its application for the eco-design of industrial processes. The second case study involves the production of synthetic fuels from biomass sources. This complex project showcases the capabilities of eco2des in providing sustainable designs and reliable insights on controversial technologies, such as those under study to decarbonize the industrial sector.

On the one hand, the first case study involves the conversion of excess wind energy into hydrogen through electrolysis, which is then reacted with carbon dioxide to produce synthetic natural gas (SNG) for seasonal storage. Furthermore, the heat produced in the reaction is recovered in a Rankine cycle which may use water or cyclopentane as working fluid. The study employs a cradle-to-gate approach with a functional unit of 1 Nm^3 of SNG and focuses on minimizing both the life cycle global warming potential (GWP) and levelized cost of production (LCOP) of SNG.

Two multi-objective optimization problems (MOOP) were solved using MOEA/D and NSGA-II algorithms, respectively. The results showed that the environmental and economic performance objectives were non-conflicting. The optimal H_2/CO_2 ratio for all scenarios varies between 4 and 4.5, with reactor temperatures ranging from 285°C to 400°C. The highest storage efficiency is achieved with a H_2/CO_2 ratio near to the stoichiometric relation, a temperature of 285°C, a reactor length of 16.83 m, and a length-to-diameter ratio of 7.92, using cyclopentane as a working fluid. However, this configuration leads to a significant increase in LCOP and GWP.

Ultimately, it is recommended to optimize the process design based on non-conflicting environmental and economic performance using a single objective optimization algorithm. This configuration achieves a LCOP of 1.48 €/Nm^3, a GWP impact of 1.09 kg CO_2-eq./Nm^3, and a storage efficiency of 57.95%, with a H_2/CO_2 ratio of 4.44, a reactor temperature of 396°C, a reactor length of 2.64 m, a reactor length-to-diameter ratio of 5.72, and water as the working fluid. A hydrogen recovery system is required, but the high carbon dioxide conversion of 98.63% allows SNG injection into the grid without further recovery.

On the other hand, the second case study illustrates the valuable insights that eco2des can produce for a complex technology under development. In the context of increasing demand for clean and renewable fuel sources, this case study focuses on the environmentally and economically optimized production of synthetic biofuels from biomass sources. The goal of this study is to environmentally and economically optimize the biomass to liquid (BTL) refinery for the co-production of synthetic biofuels and electricity, using a life cycle perspective. Following the literature, the plant size is initially set to treat 2,000 tons/day of dried biomass, but is later increased to 2,800 tons/day during the life cycle interpretation phase as the first scale is not economically feasible. The eco2des tool is employed to support this decision and the scale-up study.

The study uses the ecoinvent 3.6 version with the Cut-Off system model for background system LCA analysis and employs the present worth method for computing capital expenditures (CAPEX) and operational expenditure (OPEX) in the LCC model. A cradle-to-gate approach is chosen for the system boundaries, focusing on the optimization of process design parameters. The functional unit (FU) is defined as 1 kWh of fuels produced (hydrogen, gasoline, kerosene and diesel), and two environmental impact categories are evaluated: global warming (GW) and fossil depletion (FD), along with net present value (NPV) as a measure of economic performance.

Two multi-objective optimization problems (MOOP) are formulated: MOOP1, which aimed to minimize global warming potential (GWP) and maximize net present value (NPV), and MOOP2, which aimed to minimize GWP, maximize NPV, and maximize kerosene production. Both MOOPs were solved using evolutionary algorithms (NSGA-II for MOOP1 and MOEA/D for MOOP2). The results of these optimizations were compared with the reference case from the literature to determine the potential improvements in the biorefinery's economic and environmental performance.

The Pareto front of MOOP1 shows conflicting objectives between minimizing GWP and maximizing NPV. Lower GWP is achieved with higher electricity surplus production, while higher NPV is achieved with higher hydrogen production. Key decision variables that influenced the results include gasification temperature, steam-to-biomass ratio, GHSV (gas hourly space velocity), and H_2/CO ratio. These variables play essential roles in determining the balance between environmental and economic performance.

The Pareto front of MOOP2 reveals conflicts among all three objectives (GWP, NPV, and kerosene production). As in MOOP1, GWP and NPV exhibit similar behavior, while kerosene production is mainly influenced by GHSV. Higher kerosene production is achieved at lower GHSV values, but this compromises the economic performance due to increased hydrogen consumption for wax hydrocracking. Steam-to-biomass ratio and H_2/CO ratio also affected kerosene production but to a lesser extent.

The comparison with the reference case demonstrates that all optimized scenarios achieved better economic and environmental performance but reduced kerosene production. This comparison highlights that the current approaches for biofuels production are focused on maximizing the amount of liquid fuels, which may result in economically unfeasible plants. Co-production of hydrogen alongside liquid fuels emerges as a potential solution for improving both economic and environmental performance.

8. General discussions, conclusions and future work

The novel eco-design methodology for industrial processes developed in this research demonstrates its ability to generate optimal scenarios in process engineering, focusing on sustainable criteria. Furthermore, the eco2des tool proves to be an effective decision support system in two case studies, emphasizing its potential for holistic eco-design studies and accelerating the sustainable time-to-market for novel industrial processes.

In the methanation case study, eco2des showcases its capabilities in conducting an eco-design study using the Python tool, underlining the software's potential for holistic analysis without compromising implementation simplicity. On the other hand, the biorefinery case study illustrates the effectiveness of eco2des in a complex system, revealing that traditional process design might not be optimal in sustainable terms. This highlights the importance of adopting an integral methodology based on eco-design framework for industrial processes developed in this thesis.

It is worth to mention that the importance of rigorous and predictive models within the eco2des framework cannot be overstated, as they ensure the accuracy and validity of results. Main challenges during the tool's development include the lack of a common data interface, which hindered interoperability. Therefore, digitalization serves as a critical enabler of sustainable solutions and interoperability, paving the way for future advancements in the field. Incorporating real-time data from sensors and Internet of Things (IoT) devices, digital technologies can streamline data collection, management, and analysis, as well as facilitate collaboration and knowledge sharing among stakeholders.

To conclude, future work should focus on: Integrating Social Life Cycle Assessment (S-LCA) into the methodology to assess the whole sustainability dimensions, providing a comprehensive understanding of the social implications of industrial processes. Moreover, it should focus on developing real-time digital solutions that leverage real-time data for enhanced decision-making and process optimization, allowing for dynamic adjustments and improvements. Finally, future research should explore AI-driven predictive models based on neural network to produce the predictive life cycle inventory (P-LCI), enabling more efficient optimization and real-time decision-making by reproducing industrial process behavior with greater speed.

1. INTRODUCTION AND MOTIVATION

1.1. What is sustainability?

Sustainability means meeting present needs without compromising the ability of future generations to meet their own needs (UN 1987). Sustainability is not just environmentalism. Since in addition to natural resources, we also need social and economic resources. Therefore, sustainability is a holistic approach that considers ecological, social and economic dimensions (Figure 1), stating that all must be considered together to find prosperity.

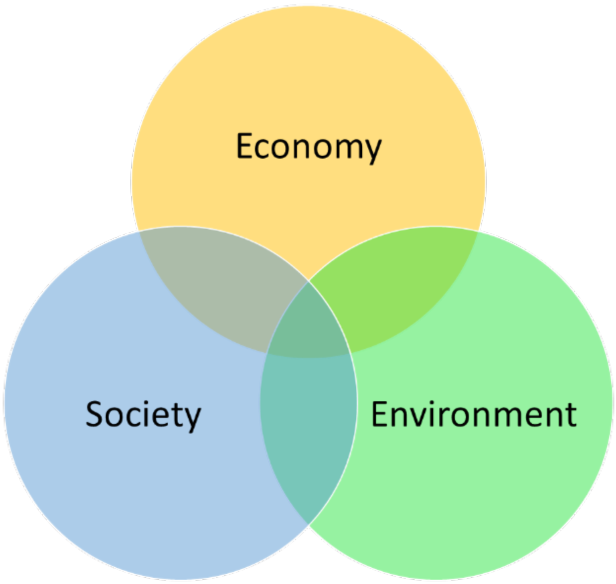

Figure 1. Three pillars of sustainability

1.2. Current sustainability context

In the last years, companies, governments and consumers have become more concerned in promoting sustainable production and consumption, improving environmental, economic and social performance with a life cycle approach including the whole supply chain (Mazzi 2020).

In this trend, life cycle thinking (LCT) has become the central concept to provide support in better integrating sustainability into the world development, from research and innovation to people demand, passing through business growth and policy making (Pennington et al. 2007). Therefore, LCT is about set aside traditional focus on production site and manufacturing processes to start considering environmental, social and economic impacts of products, systems or services over their entire life cycle (Figure 2).

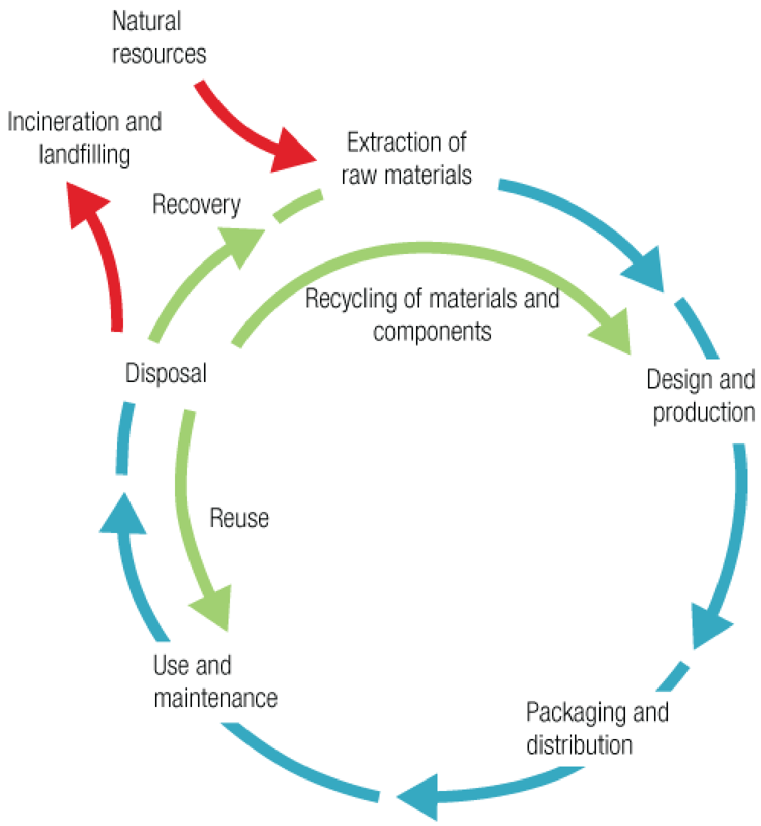

Figure 2. A typical product lifecycle diagram (LCI-webteam, 2022)

The main goals of LCT are to reduce a product's resource use and emissions to the environment as well as improve its socio-economic performance through its life cycle. This may facilitate links between the economic, social and environmental dimensions within an organization and through its entire value chain.

There is a tight link between LCT and sustainability, becoming the former, the vehicle to achieve sustainability goals. Therefore, over the past two decades, LCT has provided a conceptual basis for moving the agenda forward. As consequence, life cycle approaches and tools have been developed, refined, and are now more commonplace in the private and public sector. These have been developed to assist in decision-making at all levels regarding the product life cycle.

1.3. Life cycle approaches and tools

A life cycle approach identifies opportunities and risks of a product or technology, from raw materials to disposal (from cradle to grave). Life cycle approaches have been used for many different purposes, from day-to-day shopping, to selecting suppliers, engineering a new product design, or developing a new process, project, or business (Hertwich 2005). Therefore, nowadays, citizens, businesses, and governments are finding ways to promote LCT and to balance the impacts of their choices.

With that purpose, the scientific community and international organizations promote the use of life cycle tools, which includes standards and guidelines to assist researchers, practitioners and companies in applying the principles of life cycle thinking to product, processes and projects (Mazzi 2020).

1.3.1. Life cycle assessment

Life Cycle Assessment (LCA) is a standardized tool to evaluate the environmental burdens associated with a product, process, or activity. It identifies and quantifies energy and materials used and wastes released to the environment; with the final objective of identifying and evaluating opportunities for environmental improvements. LCA embraces the entire life cycle of a product, process, or activity, encompassing extraction and processing of raw materials; manufacturing, transportation, and distribution; use, reuse, maintenance; recycling, and final disposal (SETAC 1994).

LCA is a methodology commonly accepted and widely applied for sustainability assessment. Furthermore, it follows a well-defined procedure, described in detail in two international standards, ISO 14040 and 14044 (ISO 2006a; 2006b).

Therefore, LCA is an important decision-support tool that, among other functions, allows companies benchmarking and optimizing the environmental performance of their business or for policymakers to design policies for promoting sustainability. Hence, many LCA analysis are conducted to support internal decision-making, such as for eco-design of products, process optimizations, supply-chain management, and marketing and strategic decisions (Hellweg and Milà i Canals 2014).

1.3.2. Life cycle costing

Life cycle costing (LCC) is not a new life cycle tool. It was reported for the first time in a tractor delivery contract in the 1930s in the United States, and, further developed by the US Department of Defense in the mid-1960s for the acquisition of high-cost military equipment (Ciroth et al. 2008).

LCC is a tool to evaluate the costs associated with a product, process or activity in its whole life cycle, from its design through its production, transport, and to its end of life. Therefore, LCC can be used by private and public organizations to optimize the cost of acquiring, owning, and operating physical assets over their useful lives, trying to evaluate all the significant costs involved in the life cycle (Woodward 1997).

Furthermore, LCC is usually used combined with LCA, becoming, as well, a commonly accepted methodology for sustainability assessment. However, in contrast to LCA, LCC is not standardized in any international standard for any context. Although, the standard ISO 15686-5:2008 (ISO 2017) provides the guidelines for the application of this methodology in the building sector; it cannot be applied to other contexts.

In the literature, three types of LCC have been described: conventional LCC, environmental LCC, and societal LCC (Hunkeler, Lichtenvort, and Rebitzer 2008). First, the conventional LCC is the assessment of all the costs associated with the life cycle of a product, focusing on real, internal costs and sometimes the costs of the end of life are not included, adopting a cradle-to-gate system boundary. Then, the environmental LCC is the evaluation of all the costs associated with the life cycle of a product covered by the actors, for instance suppliers, manufacturers, users, and end of life actors. In this dimension the concept of externalities is introduced. Externalities are costs or benefits that are not reflected in the price of a product or a service. These costs are external to market transactions and, usually, affect third parties. For example, when a factory emits pollution into the air or water, it creates a negative externality because the costs of the pollution are not included in the price of the product being produced, but instead, the costs are borne by society as a whole. Therefore, the environmental problems are expressed as a one-dimensional unit, monetary flows and considered together with conventional costs and benefits (Gluch and Baumann 2004) . Finally, the societal LCC includes all the costs that are associated with the entire life cycle of a product, considering also social impact externalities. These costs are covered by anyone in the society, even in the long-term future (Hunkeler, Lichtenvort, and Rebitzer 2008).

1.3.3. Social life cycle assessment

Social life cycle assessment (S-LCA) is a novel methodology to address the social impacts of products, processes or services along their life cycle. It is based on LCA methodology, with some nuances, and was developed in accordance with the ISO 14040 and 14044 standards (Ekener Petersen 2015).

In S-LCA , social impacts are mainly understood as the impacts on human capital, human well-being, social behavior, and cultural heritage (Joint Research Centre et al. 2015). Therefore, S-LCA becomes a life cycle approach essential to cover the third pillar of sustainability along with LCA and LCC. However, the level of methodological development, application, and harmonization of S-LCA is still at a preliminary stage (Joint Research Centre et al. 2015). This way, different S-LCA methodologies have been proposed in several case studies and discussions are still open in the research community regarding the role of local stakeholders and the need of a common social theory as base to develop S-LCA (Ekener Petersen 2015). Furthermore, it is still under debate whether qualitative or quantitative assessment methods are more suitable for S-LCA, and social issues are influenced by the subjectivity of researchers and the social context (Soltanpour, Peri, and Temri 2018).

In the last years, new guidelines are under development for the application of S-LCA (Andrews et al. 2009, Benoit Norris et al. 2018), they will consider and incorporate methodological advancements based on recent practical experiences, as well as deal with harmonization of S-LCA methods.

Therefore, as the S-LCA methodology is still under discussion and development, its implementation in the framework and tool developed during the work of this thesis has been excluded. However, it will be a key point to study in future work development.

1.3.4. Life cycle sustainability assessment

As explained in section 1.1, for achieving sustainability, the environmental, economic and social aspects must be assessed and tuned against each other. Therefore, life cycle sustainability assessment (LCSA) emerged as a life cycle tool that combines LCA, LCC and S-LCA.

However, there are some prerequisites for using this technique. The most important requirement is that the system boundaries of the three assessments must be consistent, and, ideally, identical; using, if possible, the same life cycle inventory (LCI) (Kloepffer 2008).

It is noteworthy that in addition to Kloepffer definition, Guinée, taking it as starting point, added two dimensions to the evaluation, related to the external contest of organizations: technological conditions and economic state (J. Guinée 2016).

1.4. Sustainability policies

Several studies were developed to assess the level of implementation of LCT in policies (Curran 1997; Sonnemann et al. 2018), some of them focused on specific areas, such as for EU (Sala et al. 2021) or USA (Reed 2012). Among them, the European Union (EU) has been more in the forefront of applying LCT to policy development and application than any other region (Sonnemann et al. 2018; Reed 2012). For instance, European initiatives on life cycle based policies are being examples to follow for other regions such as Brazil (Maia de Souza et al. 2017).

European policies have increasingly mentioned LCT and life cycle approaches since several years ago: from the Ecolabel Regulation of 1992 (EC 1992), to the Green Deal in 2019 (CEC 2019).

Among all these European policies based on life cycle approaches or that promotes the LCT methodologies, the most relevant are: first, the communication on Integrated Product Policy (IPP) (CEC 2001) as it recognized LCT as an element that contributes to sustainable development and a scientific decision-making tool. Then, the Ecolabel Regulation (EC 2010) and the Ecodesign Directive (EC 2009) made relevant applications of LCT in policies, such as, respectively, promoting products with reduced life cycle environmental impacts and improving the environmental performance of energy-related products. An important step in the development of LCT-based policies was the communication "Building the Single Market for Green Products" (CEC 2013) and the associated regulation (EC 2013) , establishing the Product and Organization Environmental Footprint methods (PEF and OEF). These LCA-based methods seek the quantification of the environmental impacts related to products and organizations, improving replicability, robustness and transparency. Not long ago, the concept of LCT has been present in relevant policies and communications such as the European Green Deal (CEC 2019). This communication states the commitment of the EU to reach carbon neutrality by 2050. Finally, even after the COVID19 pandemic, LCT has been a key factor in European policies in order to allocate the named Recovery and Resilience funds in projects and initiatives aligned with the EU objectives towards a more sustainable economy (CEC 2020b; EC 2021).

Before closing this section, it is worth mentioning the role of the European Commission-Joint Research Centre (EC-JRC), which has been working towards promoting LCT in business and in policy making, such as in the European Platform on LCA (EPLCA) (EC 2022).

1.5. Current sustainability context in the industry

As stated during this section until now, there are several life cycle approaches and tools to assess sustainability of products, processes or any activity. Furthermore, companies, governments and consumers are demanding a more sustainable production and consumption. Consequently, the current challenge lays on how to incorporate and standardize the sustainability concept in different key sectors in order to achieve this goal and promote a sustainable development.

Among all available sectors, industry is crucial to ensure progress and prosperity. In the EU, it makes up more than 20% of the economy and employs around 35 million people, with many more millions of jobs linked at home and abroad. It also accounts for an 80%

of goods exports and is a key reason behind the EU's position as top global provider and destination for foreign direct investment (CEC 2020a).

In the industry sector, about half of total greenhouse gas emissions and more than 90 % of biodiversity loss and water stress come from resource extraction and processing of materials, fuels and food (CEC 2019). Furthermore, the production and use of energy across economic sectors account for more than a 73 % of the world's greenhouse gas emissions, being more than a 24 % of them due to the energy use in industry (World Resources Institute 2022). Therefore, industry is a key sector to achieve worldwide sustainability with a prosperous society, with a modern, resource-efficient, and competitive economy; and where there are no net emissions of greenhouse gases. All industrial value chains, including energy-intensive sectors, will have a key role to play. They will all have to work on reducing their own carbon footprints but also accelerate the transition by providing affordable, clean technology solutions and by developing new business models.

1.6. Conclusions

To achieve the ambitious objective of decarbonizing the industry sector in line with net-zero policies developed during recent years, new value chains must be studied and developed, as well as the current ones must be optimized in terms of sustainable key performance indicators. However, during the development of new innovative processes, there are no industrial data that can support any LCSA analysis, which gives rise to numerous trial-and-error phases during technology upscaling, exorbitantly increasing time-to-market and costs, while achieving solutions that may not be optimized or, even, feasible in sustainable terms.

Predictive models and process simulations, however, can compute, through physicochemical relationships, the behavior of that technology under development at industrial scale and formulate scenarios for environmental or cost optimization. Even so, process simulation, and LCA and LCC methodologies are well structured and there are many options of commercial software specialized in these areas. Nowadays, at the best of our knowledge, there is no current research combining them in a holistic way, in a unique tool, for their application in the economic and environmental optimization of any industrial design of process under research and/or development. With this premise, the current thesis you are reading was born.

2. OBJECTIVES

This thesis aims at contributing to define an eco-design methodology for sustainability-based optimization of industrial processes, combining, in a holistic way, process simulation, LCA, LCC and mathematical optimization. Furthermore, the methodology is encapsulated in a computer-based software to ease its application in future studies or projects. In particular, the main thesis objectives are:

- Reviewing the state-of-the-art of applications, methodologies and frameworks that combines predictive and descriptive models with LCA, LCC and multiple-criteria decision analysis.
- Establishing a holistic methodology for the sustainability-based optimization of industrial processes based on process simulation, LCA, LCC and mathematical optimization.
- Developing a precommercial software for the computer aided sustainability-based optimization of industrial processes based on the formulated methodology.
- Testing and validating the methodology and software.

3. STATE-OF-THE-ART REVIEW

3.1. Introduction

As new technologies are developed to answer the needs of a growing population that demands higher standards of living, concerns about the environmental impact of industrial activity continue to rise. For an enterprise to be sustainable, not only technical and economic matters need to be considered, but also how to generate the least possible environmental damage. To this end, the integration of techno-economic analysis (TEA) and life cycle assessment (LCA) has been proposed (Mahmud et al. 2021). On the one hand, TEA is a methodological approach to evaluate the technical and economic performance of a process, product, or product system (Zimmermann et al. 2020), and a common way of conducting TEA in the industry is by carrying out a process simulation together with a cost assessment such as a conventional LCC. On the other hand, LCA analyzes the environmental impacts of such product or process in a life cycle method according to relevant material and energy inputs and outputs (ISO 2006a).

Going through TEA and LCA integration for industrial applications requires comprehensive project planning since, for example, one design option may perform better environmentally while leading to financial loss. The numerous factors that must be considered to take this integration approach remain a matter of concern when policymakers, companies, or any other actor faces the need to conclusively and definitively choose between alternative solutions to a given issue. To solve this situation, possibilities are community-based decision-making, round table discussions, or even executive fiat. However, if they do not count with proper tools to interpret fundamentally conflicting information, the conclusions can significantly vary and depend on subjective factors. In this scenario, Multiple Criteria Decision Analysis (MCDA) is frequently implemented to help alleviating these problems by providing a transparent and repeatable element of decision support (Kalbar and Das 2020). See Excurse 1 to expand on well stablished MCDA methods such as TOPSIS (Hwang and Yoon 1981), AHP (Saaty 1987a), VIKOR (Opricovic and Tzeng 2004) and DEA (Charnes, Cooper, and Rhodes 1978).

Although the integration of TEA and LCA is still a recent methodological approach with no current consistent guidelines, it has indeed been implemented for the optimization of industrial processes and especially in developments of low technology readiness levels (TRL) (Mahmud et al. 2021). Decisions taken at these low stages of industrial design have a stronger impact on the final product because most harder to revert decisions are made in the early phases of technological development (Tischner et al. 2000). As a result, incorporating technology assessment tools such as TEA and LCA at low TRLs offers the advantages of optimizing economic returns while minimizing environmental damage. A variety of industries have followed the TEA-LCA integration approach for the optimization of their technological processes. Frequently, these integration methodologies are specific to a particular technology. Such application cases will be presented below.

Excurse 1: MCDA methods. Multiple Criteria Decision Analysis (MCDA) is a decision-making methodology that involves evaluating and ranking alternatives based on multiple criteria or objectives. The methodology seeks to provide decision-makers with a structured and transparent approach for making complex decisions that involve multiple, often conflicting, objectives. It incorporates both quantitative and qualitative information and allows decision-makers to consider a wide range of factors that are relevant to the decision problem. These factors can include economic, social, environmental, and technical considerations.

There are several different MCDA methods, the following are mentioned within the state-of-the-art review:

- **Technique for Order Preference by Similarity to Ideal Solution (TOPSIS)**

The TOPSIS method involves the construction of a decision matrix that contains the performance of each alternative on each criterion. The decision matrix is then normalized to remove any differences in scale among the criteria. Next, the ideal and anti-ideal solutions are calculated, which represent the best and worst performance of each criterion. The distance between each alternative and the ideal and anti-ideal solutions are then calculated, and the relative closeness of each alternative to the ideal solution is determined. The TOPSIS method assumes that the best alternative is the one that is closest to the ideal solution and furthest from the anti-ideal solution.

- **Analytic Hierarchy Process (AHP)**

The AHP method involves breaking down a complex decision problem into a hierarchy of criteria and sub-criteria, with the top-level criterion being the overall objective of the decision problem. The decision-makers then evaluate the importance of each criterion and sub-criterion relative to the other criteria, using pairwise comparisons. The pairwise comparisons are based on a scale that ranges from 1 (equal importance) to 9 (extreme importance) and are used to derive weights for each criterion and sub-criterion. These weights are then used to calculate a weighted score for each alternative, which reflects how well each option satisfies the decision criteria.

- **Vlsekriterijumska Optimizacija I Kompromisno Resenje (VIKOR)**

The VIKOR (in Serbian) method functions by maximizing the group benefits and minimizing the individual regrets. The principle of the VIKOR approach is to find the positive ideal result and the negative ideal solution at first. The positive term consists of the best value of each alternative in each evaluation criterion, while the negative term refers to the worst value of each option in each assessment criterion. Finally, the priority of each option is decided according to the degree of proximity between each evaluation value and the ideal pattern.

- **Data Envelopment Analysis (DEA)**

The DEA method is a non-parametric Multiple Criteria Decision Analysis (MCDA) method used to evaluate the efficiency of decision-making units (DMUs) that use the same inputs to produce the same outputs. It involves the construction of a decision matrix that contains the performance of each DMU on each input and output. The method then determines the relative efficiency of each DMU by comparing its performance with that of the other DMUs. DEA uses linear programming techniques to construct an efficient frontier that represents the optimal combination of inputs and outputs for each DMU. Finally, the method then calculates the efficiency score of each DMU.

- **Multi-objective genetic algorithms (MOGA)**

The use of MOGA methods is a quantitative MCDA that involves the use of a genetic algorithm to search for the optimal solution among a set of alternatives that satisfy multiple objectives. This method uses a population of potential solutions that are evaluated based on their fitness to the decision criteria. The solutions with the best fitness are then selected for reproduction, and the process is repeated until a satisfactory solution is found.

3.2. Applications of integrated TEA, LCA and MCDA

This state-of-the-art review section aims to explore the application of integrated TEA, LCA, and MCDA methodologies in the industrial sector and demonstrate their potential benefits and versatility.

Two promising and innovative sectors, biofuel production pathways and carbon dioxide revalorization, have been selected as key areas of focus in this review since they are targeted during the case studies development. The biofuel industry has experienced significant growth and innovation in recent years, driven by the global demand for cleaner and more sustainable energy sources. Carbon dioxide revalorization, on the other hand, has emerged as a critical area of research due to the urgent need to mitigate greenhouse gas emissions and develop effective carbon capture and utilization technologies. By examining the integration of TEA, LCA, and MCDA in these sectors, this review seeks to highlight the potential of these methodologies in supporting sustainable development and fostering technological advancements.

In addition to these emerging sectors, a more mature industry, water treatment, has also been included in this review. Water treatment is a well-established sector with considerable historical and practical knowledge. Including this sector allows us to explore the effectiveness of the integrated approach in optimizing existing technologies and identifying areas for improvement, thus demonstrating the relevance of TEA, LCA, and MCDA integration across different stages of industrial development.

Furthermore, this review encompasses other relevant applications of the integrated approach in various industrial sectors to demonstrate the wide applicability of the methodology. By examining these diverse examples, the review aims to showcase the versatility and adaptability of TEA, LCA, and MCDA integration, offering insights into its potential for driving sustainability and innovation across a broad range of industries.

3.2.1. Biofuel production pathways

From a multi-objective optimization perspective, Wang and coworkers (L. Wang et al. 2010) conducted a TEA-LCA integration for the development of bio-refinery gasification pathways. Their methodology involved multi-objective superstructure optimization and mixed integer nonlinear programming (MINLP). In their model, they evaluated economic performance and environmental effects as the two-process behavior indicator. To measure economic outcomes, they used the Net Present Value; for environmental impacts, they studied the Global Warming Potential (GWP). After analyzing the resulting Pareto-optimal curve, which displayed all design solutions for optimal processes, an improved understanding of the transactions between economic and environmental facets of the biorefinery was reached. Thorough mathematical modeling was performed to elucidate MINLP using GAM 23.8.1 (Tawarmalani and Sahinidis 2005); however, this procedure was considered very problematical and time-consuming. The final optimized design still needed adjustments as significant amounts of greenhouse gases (GHG) emissions were reported. In a later study, carbon capture remodeling was considered a potential methodology for fixing the results (Davis et al. 2013).

Algae-based biofuel production has also been studied through the integration of TEA and LCA. Using a multiple-objective approach, the Cornell Marine Algae Biofuels Consortium was operating on 20 production processes in 2015, all of which were considered case studies (Beal et al. 2015). Here, researchers contrasted these processes for most and least advantageous in terms of economy, energy, and green care by pondering five environmental impact categories, capital and operating costs, and energy return on investment (EROI). While implementing TEA-LCA as a design tool, they used the results of one process scenario to report design options for subsequent iterations, which is essential to avoid recommending environmentally friendly strategies that are not lucrative and vice versa. Unfortunately, the results of which process design parameters deliver the best outcomes across the different categories were not reported.

The National Renewable Energy Laboratory (NREL) of the United States of America (USA) has also undertaken efforts to integrate TEA and LCA for production from algal sources. In this case they also integrated Resource Assessment (RA). Their objective has been to evaluate the generation of renewable diesel from algal lipids by harmonizing the results of each of these models separately. For this purpose, the Aspen Plus simulator (Haydary 2019) was employed for conducting TEA, while the GREET model (M. Wang et al. 2020) was incorporated for conducting LCA. Sensitivity analyses were performed on both TEA and LCA outcomes, followed by systematic harmonization to obtain an integrated result that considered costs and environmental impact. This harmonization for integration was not simultaneous and no changes were applied to the process parameters for optimization. The results of this work, evaluated in Davis et al. (2013), offer a quantitative framework for weighing progress and gaps in algal biofuel development. Nevertheless, this framework has some uncertainties related to the harmonization process and the shortage of publicly available data.

Following the subject of biofuels, DeRose (DeRose et al. 2019) performed a multi-objective analysis that integrated TEA and LCA for the transformation of high-productivity, low lipid algae to renewable fuels. For this purpose, TEA was conducted by combining process and economic models, while LCA was performed by linking model material and energy balance data. In particular, the energy records were obtained from the NREL LCI database (NREL 2012) and involved net GHG emissions. Conversion processes were modeled by the Aspen Plus software, while the optimization problem was focused on minimal fuel selling price and global warming potential. In line with this, a discounted cost flow rate of return evaluation was implemented to calculate the minimum fuel selling price, or levelized cost of production (LCOP).

Wu, Lin and Chang (Wu, Lin, and Chang 2018) also implemented a TEA-LCA integration to design an optimization model that delivered the best combination of cultivation and pretreatment process chain for an algal biorefinery. This optimization model was intended to minimize environmental impact and maximize profits. Using TEA and LCA standards, microalgae-to-biofuels chains for the simultaneous production of diesel and ethanol can result in desirable investment circumstances and low environmental impact. In this project, the heat recovery scheme, the entrained recovery tower, and CO_2 recycling were essential parts of the design. Here, the authors solved a specific optimization algorithm that considered 180 equipment combinations and different lipid content of microalgae. After implementation, this integration model promoted the reduction of life cycle GHG emissions. They concluded that this optimization methodology allowed them to determine the optimal combination of cultivation and pretreatment practices in the microalgae-to-biofuels chain.

The optimization of algal biofuel production was also analyzed under a TEA-LCA integration by Hise et al. (Hise et al. 2016). This study was conducted on the conception that the value of technical progress is subject to modeling assumptions regarding growth conditions, process design, and funding of the industrial facility into which novel methods are incorporated. In this sense, two related techniques, algal growth and dewatering were assessed in representative operating and financing situations. TEA-LCA integration system analysis was chosen for its capacity to provide estimates of facility economic competitiveness (Zhu et al. 2013), life cycle environmental impacts, and elucidate the production risks that constitute barriers to investment (Miller et al. 2013). The authors aimed to address previously unexplored connections between technical improvements and financial parameters, and study how tradeoffs resulting from these interactions influenced the cost competitiveness of an optimal facility design. Therefore, in their developed TEA/LCA model, they evaluated performance benefits that proceeded from the use of reported techniques for (1) increasing lipid productivity with a bicarbonate amendment (Lohman et al. 2015) and (2) reducing capital costs and energy efforts for dewatering by implementing temperature-sensitive “hydrogels” (Vadlamani et al. 2014). These techniques were evaluated in a pathway perspective by means of either transesterification or hydrothermal liquefaction (HTL) conversion techniques, and through a range of attainable algal lipid content and growth rates, in order to measure the influence of these working factors on the relative benefits of incorporating novel techniques. The results of this project suggested that these technologies could be valuable under specified conditions, but also that investment subsidies influenced cost-competitive facility design by incentivizing the development of more capital-intensive facilities (e.g., favoring hydrothermal liquefaction over transesterification-based facilities).

Integrated TEA and LCA have also been used to optimize integrated wastewater treatment and microalgae production for biodiesel generation from an early design stage (Barlow, Sims, and Quinn 2016). In this case, a model was constructed modularly to support the assessment of alternative sub-processes and various scenarios, including the sustainability of producing renewable diesel by means of hydrothermal liquefaction (HTL) of biomass using a rotating algal biofilm reactor. Pilot-scale development analysis and laboratory-scale HTL experiments were conducted to validate an industrial system model. Once, validated, this model became the foundation to estimate the economic viability and environmental impact of the system at a full scale. Posterior scenarios evaluated the integration of wastewater treatment and the optimization of system performance parameters. The study exhibited the performance of the model for generating renewable fuels in terms of global warming potential, net energy ratio, and economic indicators. Finally, the combination of algae cultivation with wastewater treatment was found to significantly decrease environmental impact. Moreover, sensitivity analysis showed that fuel selling price was mostly influenced by algal output, which highlighted the importance of optimizing biomass productivity.

Finally, regarding the efficient use of biomass resources, integration of TEA and Territorial Metabolism Life Cycle Assessment (TM-LCA) (Sohn, Vega, and Birkved 2018) has been proposed to reach the highest environmental and economic gains for a given region (Croxatto Vega et al. 2020). To reach this objective, three biotechnology alternatives for anaerobic digestion (AD) were evaluated at two different scales (200 kW and 1 MW of installed electric capacity) in two different regions. In the first place, environmentally friendly feedstock accessibility for two European regions was measured. Secondly, an investigation was conducted to determine the environmental effect and financial potential of each technology when scaled up to the regional level, considering all the area's unique sustainably feedstock available. To obtain regional single scores for the assessments, MCDA and internalized damage monetization were applied. The most suitable technology scenario producing the highest amounts of energy was determined for all regions and scales. The bioplastic production was found the less preferable as the value of the produced bioplastic products was not significant enough to counterbalance the resultant drop in energy production. In conclusion, the assessments of different alternatives in a regional context supplied valuable information about the impact of different sorts of feedstock on environmental performance.

3.2.2. Carbon dioxide revalorization

In 2021, a Multi-Attribute Decision-Making (MADM) approach that combined LCA-TEA outputs was employed to rank four distinct renewable energy sources for the generation of methanol from CO_2 (McCord et al. 2021). The objective was to design a "first of a kind plant" by roundly considering the environmental effect of production, economic viability, and production scale. The energy sources (offshore wind, onshore wind, solar photovoltaic power, and geothermal power) were evaluated and ranked in order of predilection to select the most viable for development. Regarding indicators, 11 were included for the environmental analyses and 3 for the techno-economic assessments. The environmental indicators were taken from the CML LCA method (Gabathuler 2006), which calculates the dimension of the environmental impact caused by a product due to human toxicity, eutrophication, ionization radiation, and aquatic ecotoxicity. On the other side, the techno-economic indicators were overall plant Capital Expenditure

(CAPEX), Operating Expenses (OPEX) related to electricity provision, and scale of production. For the LCA-TEA integration, an Analytical Hierarchy Process (AHP) methodology (Saaty 1987b) was implemented. The results showed that even with a high number of sub-criteria, the combination of LCA-TEA outputs can be used to assist in industrial decision-making.

Among the cases where a combined TEA and LCA have been applied to optimize new production directions from an early design phase, there is the integration of Power-to-Gas technology (PtG) of methane and photovoltaics (Collet et al. 2017). PtG technology entails using electricity to transform water into hydrogen via electrolysis, and then synthesize methane from hydrogen and carbon dioxide. In this study, TEA-LCA of methane production by the combination of anaerobic digestion and PtG technology has been conducted for sewage sludge valorization. Here, the authors proposed a model for CH_4 production from PtG that assessed two dimensions of sustainability (environmental and economic). The economic assessment was performed by calculating CAPEX and OPEX for each analyzed configuration as in de Boer et al (de Boer et al. 2014). Other authors had also previously reported economic assessments of methane production from PtG (Götz et al. 2016), with the seldom use of a time-dependent optimization approach (Rivarolo, Magistri, and Massardo 2014). The environmental evaluation involved LCA as the standardized tool to measure the environmental impacts of the whole cycle of a process; precisely, from raw extraction to final waste management. Sensitivity analyses were included with a focus on biogas upgrading tools, electricity prices, annual operation time, and composition of the electricity mix. A comparison between PtG and direct injection of methane from biogas was also performed. The results suggested that the higher the prices of electricity, the longer the operation time of the methanation procedure must be to compete with the injection. Moreover, the reduction of electricity consumption during the electrolysis step decreased production costs. After this research, the authors concluded that even if the present context does not offer adapted circumstances to guarantee an economically feasible chain, the evolution of the energy perspectives in the next few years as well as the projected technological improvements will contribute to global cost reduction. From an ecological point of view, continuous PtG causes more greenhouse gases than direct injection;

however, intermittent operations using renewable electricity when it is available can considerably reduce GHG emissions. From an endpoint effect perspective, the impact from constant PtG is higher than biogas upgrading although much inferior to fossil energy.

3.2.3. Water treatment

Cost versus environmental impact optimization within an integrative assessment has also been applied to the potable water plants (PWPs) production area (Florin Capitanescu et al. 2016). The application of the LCA to the design of PWPs is frequently boycotted by: (1) a wide variety of unit processes, (2) elevated variability of the operation conditions concerning water quality input, and (3) the array of possible technical solutions to meet the treatment needs. To reach consistency in the prospective assessments, LCA should be based on running simulations of the unit processes rather than on average information, which is the most usual case when there is no real data available. In this regard, an integrated and adaptable process modeling-life cycle assessment (PM-LCA) tool for the design and LCA of water treatment was presented: EVALEAU (Mery et al. 2013). It was developed in Umberto® (v5.5) (iPoint 2022) using the Python language for code scripting, and the design was structured on a library of unit process (UP) modules. Moreover, the simulator was linked to the ecoinvent database for the life cycle inventory (LCI) of background developments. It was also designed to rely on the software PHREEQC (Parkhurst and Apello 2014) for water chemistry calculation. The input data to be analyzed in the PWPs was design, operation parameters, and water composition; also, literature or user-defined values were included. After module combination, water treatment chains could be planned and evaluated in Umberto with an elevated level of detail and specifications. The authors also included a sensitivity analysis toolbox from the Morris method (Morris 1991) to identify the process variables that would be mainly influencing the impact results. They concluded that the EVALEAU tool can successfully elucidate the challenge of connecting the LCA results to the corresponding technology design choices, including the assessment and eco-design viewpoints.

In another paper, the same author (F. Capitanescu et al. 2016) sought for further optimal solutions regarding cost and environmental aspects of PWP. Here, the researchers realized this objective constituted a constrained optimization problem with a computationally expensive process-modeling that had to be solved with limited computational budget. As mathematical programming methods were impracticable in this case, the authors proposed as a solution six existent state-of-the-art global meta-heuristic optimization algorithms suitable for such simulation-based work and evaluated their performance. These algorithms were: Particle Swarm Optimization (PSO) (Kennedy and Eberhart 1995), Differential Evolution (DE) (Price, Storn, and Lampinen 2005), Multi-Objective Evolutionary Algorithm based on Decomposition (MOEA/D) (Zhang and Li 2007), Indicator-based Evolutionary Algorithm (IBEA) (Zitzler and Künzli 2004), Non-dominated Sorting Genetic Algorithm (NSGA-II) (Kalyanmoy Deb et al. 2000), and the Strength Pareto Evolutionary Algorithm (SPEA2) (Zitzler 2002). As a result of this optimization methodology, satisfactory reduction in both functioning cost and environmental impact could be obtained. In particular, NSGA-II outperformed the other assessed algorithms.

Concluding with the potable water area, Ahmadi and Tiruta-Barna (Ahmadi and Tiruta-Barna 2015) introduced a new tool that integrates Process Modelling, LCA, and Multi Objective Optimization (a PM–LCA–MOO tool). This model was created to solve several impediments of the eco-design of conventional potable water production processes, namely the high variability of operating conditions (subject to the inlet and the quality of outlet water), and by the wide diversity of viable technical solutions and treatment processes. With the aim of connecting conflicting LCA data, the system used an already developed library of unit process modules that produces water treatment inventories (the above explained EVALEAU tool) (Mery et al. 2013). For the MOO, a hybrid (this is, local–global) derivative-free algorithm was selected. This algorithm featured: 1) the elitist NSGA-II for the initial global search towards the most promising optimal zones; and (2) the COBYLA algorithm (Powell 1998), which started with the final solutions of NSGA-II, with the aim of improving accuracy in a reasonable calculation time. The PM–LCA–MOO tool was effectively applied in a test bed case on an existing potable water plant from the Paris region. This resulted in a set of alternative solutions called “global

Pareto-optimal front" that inter-evaluates different objectives. Such objectives were to minimize environmental impacts via the ReCiPe method (Huijbregts et al. 2016) according to ISO 14040, to lower operational costs, and to maximize produced water quality.

3.2.4. Other industrial sectors

Continuing with other relevant applications, TEA-LCA integration was applied to optimize polyphenol extraction from red wine pomace (Croxatto Vega et al. 2021). Here, LCA was applied at an early design phase to attain a preliminary carbon footprint (CFP) of the polyphenol extraction methods. Later, the design of the laboratory extraction processes was improved and adapted to industrial scale, and a TEA of the industrial scale scenarios was performed. Then, to obtain a holistic picture of the economic viability and potential environmental impacts of each polyphenol extraction method, LCA was applied one more time with all environmental indicators in simulated industrial conditions. Finally, MCDA was applied with the aim of deciding between the polyphenol extraction methods and a weighting profile derivation method (Sohn et al. 2020). The criteria from both LCA and TEA were integrated to obtain concise decision support for selecting one of the laboratory methods for scale-up. For this purpose, the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) (Hwang and Yoon 1981) of MCDA was used. This case study demonstrated how early design calculations, and combined LCA and TEA can be integrated to advance process design.

Life cycle costing (LCC) is a further methodological framework that evaluates economic feasibility. TEA is compared to conventional LCC, but mainly applied in process engineering, while LCC aims to assess any product, process or service. In this regard, LCC-LCA integration has been incorporated in the optimization of numerous industrial applications. López-Andrés et al. (López-Andrés et al. 2018) investigated the environmental impacts of chicken meat production in a cradle to slaughterhouse (also called Poultry Processing Plants, PPP) perspective. With the aim of complementing LCA and delivering a more holistic picture of the system, process simulation and artificial intelligence were applied in the system. The Monte Carlo simulation implemented permitted the quantification and propagation of variability and uncertainty into the LCA results, while Artificial Neural Networks (ANN) (Livingstone 2008) and Stepwise Multivariate Regression (SMR) (L. Wang et al. 2010) were used to assign impacts without any restriction in units of measurement. Afterwards, the IMPACT 2002 + method (Jolliet et al. 2003) was used to determine the global impact using ecoinvent (Frischknecht et al. 2005) and LCA Food databases (Peano et al. 2012). Three impact allocation techniques (neural networks, mass method, and stepwise regression) were tested, and both classical and alternative allocation procedures were compared. Lastly, a multi-objective optimization model based on a Genetic Algorithm (GA) was included to create alternatives of optimal process parameters in order to lower ecological impacts in the system per Functional Unit (FU). This model considered all technical, economic, and environmental aspects. In particular, the GA addressed the difficulties caused by both the non-linear characteristic of a system and the multiple criteria assessment. In the end, the selected alternative accomplished a reduction of 15.14% per FU at the environmental indicators. In conclusion, the results encourage including support techniques for LCA (GA in particular) to conduct a reliable evaluation and an environmental/economic system optimization.

Within the tourism resort industry, enhancing the efficiency of renewable energy systems presents a complex challenge that requires a multi-criteria decision analysis (MCDA) approach. Zheng and Wang (Zheng and Wang 2020) presented a three-part evaluation criteria system that involves economy, technology, and environment, and nine sub-criteria for the renewable energy scheme. To calculate the weights of each criterion, they employed the AHP method. Finally, the VIKOR method was adopted to study the proposed energy schemes. The authors concluded that VIKOR allowed the securing of satisfactory compromise solutions for decision-makers in the industry by maximizing group benefits and minimizing individual regrets.

To conclude the review of integrated applications, Khoshnevisan et al. combined multi-objective genetic algorithms (MOGA) (Murata and Ishibuchi 1995), LCA, and data envelopment analysis (DEA) (Cook and Seiford 2009) with the aim of decreasing the environmental impacts of watermelon cropping systems (Khoshnevisan et al. 2015). Three impact categories were chosen for evaluation: respiratory inorganics (RI), global warming (GW), and non-renewable energy use (NRE). The results revealed a reduction of 27% in RI and 35% in GW and NRE if an appropriate combination of resources was applied in the watermelon production. Moreover, the implementation of LCA-DEA indicated that all three categories could be reduced by 8% if all farmers worked on the efficient frontier proposed by the authors.

3.3. Frameworks for integrated TEA, LCA and MCDA applications

After reviewing various application instances that integrate TEA, LCA and MCDA; the analysis of the integration approaches discloses a lack of consistency in criteria and methodology. As a result, there is no formal guidance for those who attempt to select a suitable integration procedure for diverse objectives. Therefore, a review of frameworks that aim to integrate these methodologies has been conducted.

In this context, Wunderlich et al. (Wunderlich et al. 2021) presented a framework that offers a systematic pathway for TEA-LCA integration through three main parts. Part I sets the key variables of the integrated evaluation (goal and scope, impact calculation, inventory data, and interpretation) in a four-phase procedure that links the results from TEA and LCA. Part II considers a variety of integration approaches (reporting vs integration) and creates three integration types based on different perspectives: qualitative discussion (Type A), quantitative combined indicator (Type B), and quantitative preference (Type C). Finally, part III consists of guidance to decide on integration approaches through a step-by-step technique that ponders the assessment purpose and the limitations that technology maturity and resource availability may impose. The three-part nature of this framework was based on the authors' conception that there is no one-size-fits-all answer for TEA-LCA integration that could serve all purposes through the phases of technology development. Further studies will be able to establish whether this framework helps grow the number of integrated studies by guiding practitioners in tailored assessments.

For its part, the Multi-Objective Multi-Technology (MOMT) evaluation framework is an approach that streamlines the traditional TEA while integrating new evaluation aspects of LCA (J. Li, Feaster, and Kohler 2019). Greenhouse emissions, sustainable goals, logistics, manufacturing, and further indicators are included in this assessment. The implementation of MOMT involves: (1) the evaluation of multiple process objectives, including profitability, energy efficiency, product quality, sustainability, environmental impact, and safety, among others; (2) the assessment and comparison of traditional and novel process technologies according to those multiple objectives with traceable practice and consistent criteria, (3) a comprehensive screening and optimal design at an early stage of the core development. To facilitate simulations while following this framework, the software AspenTech HYSYS, AspenTech Icarus (AspenTech 2022b), CAPCOST (Turton et al. 2018), GREET (M. Wang et al. 2020), and PROII (AVEVA 2022) were utilized. In particular, MOMT has been reported to allow the (1) evaluation of all types of technologies, (2) sensitive analyses of key parameters in design, (3) optimal process design through a case study or multi-objective optimization (J. Li, Feaster, and Kohler 2019). This framework could provide comprehensive evaluations for novel sustainable processes with environmental or social merits and allow the comparison with rather traditional processes using the same platform, however, the environmental indicators does not consider the whole value chain focusing on onsite emissions.

Furthermore, Thomassen et al. (Thomassen et al. 2019) introduced a prospective environmental techno-economic assessment (ETEA) framework that integrates TEA and LCA. ETEA was developed to solve the need for a framework that could apply to different TRLs. In this regard, a continuum is assembled through the progression of the technology: first, a screening ETEA is conducted at a low TRL stage; then, a streamlined ETEA takes place at middle TRL; finally, a full-scale ETEA is conducted at high TRL. Based on the characteristics of the TRL, the framework offers streamlining methodologies for LCA and TEA. This system uses modules that are specific to a technical process and are part of the superstructure of interchangeable units. As a result, optimization is facilitated because the user does not have to calculate all potential process designs; instead, only the modules are measured. As this proposed framework can determine environmental and economic hotspots from an early stage of technology development, it empowers the research to lower both environmental impacts and economic costs.

Concluding with framework developments, the German Oko-Institut has developed a framework for eco-efficiency analysis that is based on the integration of LCA and LCC. This method examines different alternatives that satisfy a defined consumer need, from an environmental and an economic point of view (Rüdenauer et al. 2005). Like LCA, eco-efficiency analysis allows the settlement of priorities in purchasing decisions, while this method can also reveal optimization possibilities in product development processes. The LCC analysis results in a single figure, which is the total cost of ownership to one or several participants. On the other hand, the environmental impacts can be calculated through two different options: (1) aggregated as a single score, or (2) each impact category results are kept separate. In either situation, two single scores can be contrasted: the total environmental load or the impact indicator results of a category, and the total costs of ownership of the options under study. By plotting the results in two-dimensional graphs, the effectiveness of a certain measure from environmental and economic perspectives can be depicted. Regarding efficiency, it is conveyed as a numerical ratio of ecological savings to the difference in costs. The impact categories that are commonly considered in the eco-efficiency analysis are Global Warming Potential (GWP), Acidification Potential (AP), Aquatic Eutrophication Potential (aEP), Terrestrial Eutrophication Potential (tEP), and Photochemical Ozone Creation Potential (POCP). Although quite similar methods have been used by other institutions, the present approach by the Oko-Institut offers greater flexibility for the practitioners in some respects. For example, in terms of the following choices: kind of alternatives to be compared, assessed impact categories, and depiction of the results; moreover, it allows the usage of different methods for pondering and aggregating the results of the categories of environmental impact. In conclusion, eco-efficiency analysis broadens the foundations for decision-making processes while it provides particularly detailed results about additional benefits and potential barriers.

3.4. Conclusions

The integration of methods such as LCA and LCC (including TEA), can be most considered a valuable contribution to quantitative assessments that include sustainability. Prospective applications of process simulation, LCC and LCA can assist technology developers in understanding the implications of different design choices on future performances (including technical, economic, and environmental) of emerging industrial processes, especially at low TRLs. This can help to reduce costs, elude environmental consequences, and prevent unfortunate investments by supporting technology designers to optimize different parameters without major disturbances. Moreover, an integrated TEA-LCA tool can also decrease inconsistencies between system boundaries, working units, and assumptions that can be present after using separate TEA and LCA findings during decision-making (Moni et al. 2020).

Despite the convenient features, until very recently most studies that have conducted TEA (or simulation plus LCC) and LCA have included them separately. In some cases, efforts have been made to harmonize separate economic and environmental results to provide insights into those results to decision-makers. Understanding the interchange between economic and environmental performances is critical for sustainable process design, which is not fully possible if these analyses are performed individually. In contrast, the integration of process simulation, LCC and LCA allows a systematic analysis of the interactions between technical, economic, and environmental outcomes and offers more information to technology designers for taking reliable decisions.

Worth mentioning, there is still a lack of consistent guidelines to perform integrated simulation, LCC and LCA in the literature which demands further methodological development. However, an increasing number of practitioners are incorporating combined TEA-LCA to assess the environmental and economic aspects of implementing new technologies and to perform multi-objective optimization to optimize process pathways. Therefore, an integrated methodology provides a gateway to finding production hot spots and openings for optimization at early design stages. In this way, scientists prefer multi-objective optimization over MCDA when integrating process simulation, LCC and LCA. Due to its quantitative nature, its ability to handle a larger number of criteria and non-linear relationships, and its ability to generate a diverse set of optimal solutions.

On the other hand, there is also a growing interest in the prospective application of integrated TEA and LCA tools to assess emerging technologies at early TRL. However, these are focused on a specific industry lacking interoperability in the wide process engineering field. Anyhow, as the integration of process simulation, LCC, LCA and mathematical optimization is still an evolving area, further exploration is yet needed to prepare consistent methodological guidelines.

Overall, an integrated methodology can evidently benefit technology developers in the creation of sustainable processes. The application of this methodology allows the simultaneous evaluation of economic and environmental viability, as well as process optimization in terms of the lowest production cost and lowest environmental impacts. Furthermore, an integrated tool that encapsulates the new methodology will speed up its adoption and development for its application to any industrial process. To sum up, as the implementation of integrated process simulation, LCC, LCA and mathematical optimization approach is expanding, further research is required to provide a consistent framework and tools that will benefit both technology developers and policymakers.

4. MATERIALS AND METHODS

4.1. Process simulation framework

4.1.1. Background

Since its beginnings in the 1970s, process simulation has undergone a considerable development. In both steady-state and dynamic modes, it is now possible to accurately model and simulate very large processes, even process networks with complicated substances behavior. This covers a wide range of unique processes, such as those from biotechnology or polymer technology, in addition to more traditional chemical processes. Therefore, process simulation has established itself as a reliable and essential tool in the creation, design, and optimization of chemical processes as a result of these wide-ranging capabilities (Sönke Bröcker et al. 2021).

4.1.2. Simulation approach

The main steps of a simulation workflow are encapsulated in a loop, which is followed until a reliable process design is reached. Figure 3 shows the simulation iterative process for a steady-state problem.

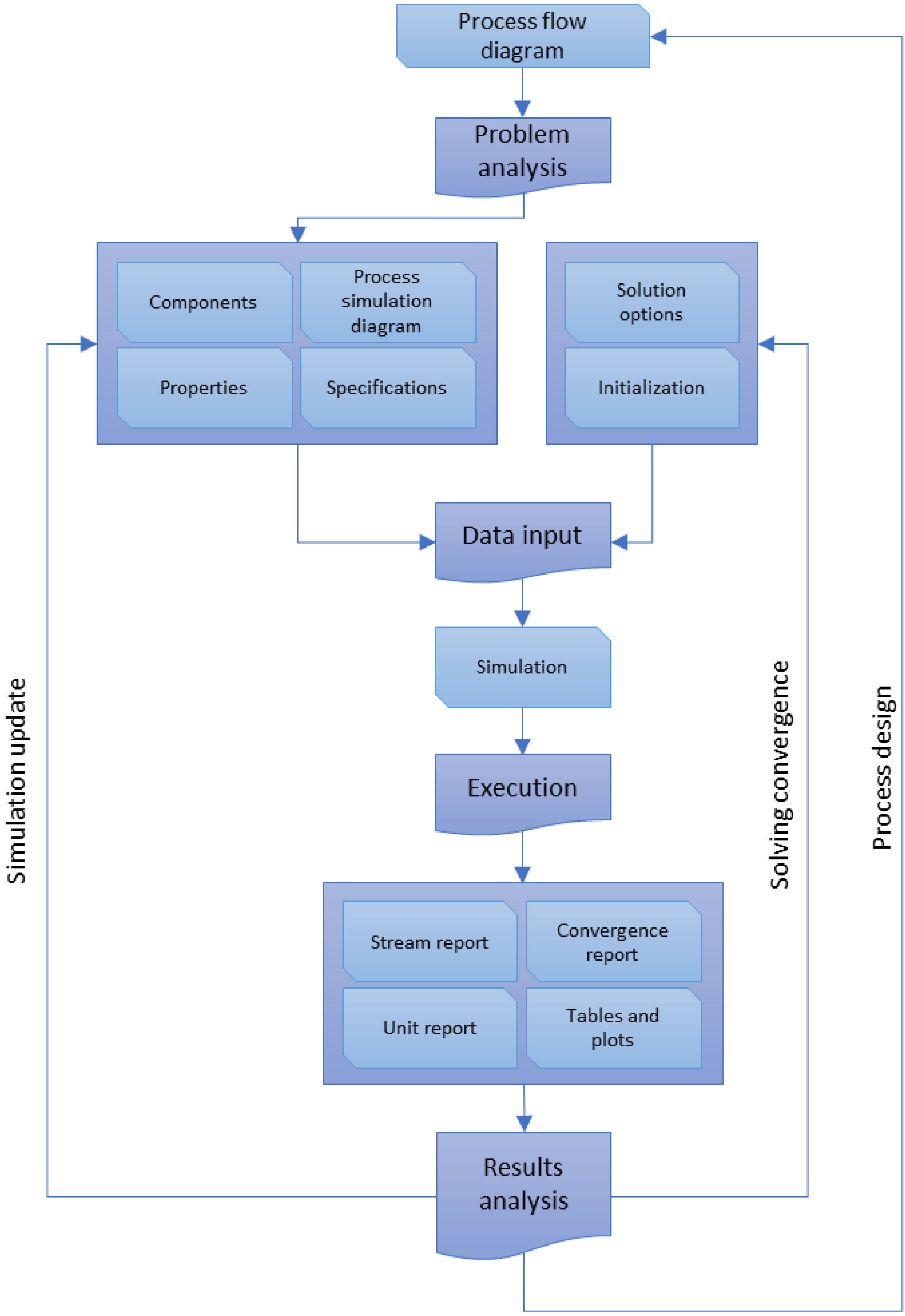

Figure 3. Simulation approach in steady-state problems (Based on (Dimian, Bildea, and Kiss 2014, 2))

4.1.2.1. Problem analysis

The starting point is a real process flow diagram that must be adapted to the software capabilities and the simulation goals, to generate the process simulation diagram. It is the flowsheet scheme developed for simulation purposes; therefore, it might be different than the process flow diagram. For example, simple units may be modelled together in a single simulation unit or, on the other hand, complex units such as distillation columns or chemical reactors, might need several simulation units to mimic their behavior. Considering that, a preliminary problem analysis is necessary with the following sub-steps:

- Examine the chemistry to determine the elements that should be included in the simulation.
- Convert the process flow diagram in a process simulation diagram.
- Determine the proper thermodynamic model (or models) by analyzing the process conditions.
- Analyze the degrees of freedom of the flowsheet and adjust, if necessary, with design specifications.

4.1.2.2. Data input

How the data input is carried out depends on the software used for developing the simulation. Usually, this step is supported by a graphical user interface (GUI) in one of the available commercial software for process engineering. However, this activity might be carried out in excel sheets or scripts as well.

Regardless of the tool used, input data are available from the problem analysis stage or from convergence options. From problem analysis the following inputs are collected:

- Choose the components from a standard or user defined database.
- Select the thermodynamic models and fine tune the model parameters.
- Draw the process flowsheet.
- Identify and define the data of the input streams.

- Analyze the degrees of freedom defining the system units.

Finally, the inputs related to the convergence options are:

- Determine the computational sequence.
- Choose the computation strategy (algorithm).
- Provide good initial data for the tear streams.
- Specify the convergence criteria.

4.1.2.3. Execution

Once the convergence criteria at both, the flowsheet, and the unit level, is satisfied; the simulation is considered successful. Otherwise, after analyzing the simulation logs a step back must be taken to update the input data for solving convergence problems.

There are several results coming from a simulation, among them the most relevant are:

- Stream report: Material and energy balances, and flowsheet convergence report.
- Unit report: Material and energy balances, and unit convergence report.
- Unit performances.
- Physical properties.

Different formats for the graphical presentation of results are possible. Advanced software typically comes with its own analytical tools, although data can also be exchanged with general-purpose spreadsheets. Furthermore, detailed results, such as internal flows or property tables, may be exported to another specialized software.

4.1.2.4. Results analysis

The first step is to validate the convergence and the reliability of the results.

On the one hand, if the simulation converges, user must verify the mass and energy balances, revise the flow rate of recycle streams, and, finally, check the product streams.

On the other hand, if the simulation does not converge or the results are unreliable, user must go through the convergence logs, errors but also warnings, in order to find out the main reasons for lack of convergence. Then, the following actions may be followed in order to solve the problem:

- Revise the components specifications and the properties calculation methods.
- Consider the possibility of using simpler but more flexible and robust models.
- Examine the requirements while keeping the entire flowsheet in mind. Avoid defining the process-outlet streams in general. Set forth the product to feed ratios or recycle flow rates instead.
- Build the flowsheet gradually and check the results after each new addon.
- Check the initial data of the tear streams or difficult system units.
- Check the convergence parameters and algorithms and make any necessary adjustments.
- Check the variable bounds.

Once the user is confident that reliability have been obtained, flowsheeting analytical tools may be used to extract more value from the simulation results. The sensitivity analysis is the most popular. Typically, this entails logging changes in a few "sampled variables" as a result of "manipulated variables." Results interpretation can be directly utilized as trends, correlations, or pre-optimization. To study scenarios of various flowsheet variables, case studies can be conducted. Finally, multi-variable optimization may be used to improve the simulation task. As a result, a new simulation cycle may begin once the designer suggests modifications or changes to the initial process flow diagram.

4.1.3. Aspen Plus

There are several major integrated simulation systems commercially available. Among them, the leading process simulation software is the Aspen ONE engineering suite (AspenTech 2022b). This is an integrated system for computer assisted process engineering, including flowsheeting systems and specialized packages. Belonging to this suite, Aspen Plus (AspenTech 2022a) is a steady-state simulation environment which includes a comprehensive database and several thermodynamic models. It is frequently used for process design and techno-economic analyses in the chemical industry, but also in biofuel processes and power plant engineering (Haydary 2019). Therefore, it is the commercial software chosen for the development of this thesis.

4.2. Life cycle assessment framework (LCA)

4.2.1. Background

As explained in section 1.3.1, LCA is a standardized methodology commonly accepted and widely applied for the evaluation of the environmental burdens of an industrial process. It identifies and quantifies energy and materials used and waste released to the environment; as well as their impacts associated; with the final objective of identifying and evaluating opportunities for environmental improvements. LCA embraces the entire life cycle of a process, encompassing extraction and processing of raw materials; manufacturing, transportation, and distribution; use, reuse, maintenance; recycling, and final disposal (SETAC 1994).

4.2.2. LCA approach

As a standardized methodology, LCA follows a well-defined proceeding, described in detail in two international standards 14040:2006 and 14044:2006 (ISO 2006a; 2006b). The elaboration of an LCA study is an iterative process and requires the collection of huge amounts of data. The main process steps of any LCA study, as applied also within this thesis, are shown in Figure 4 and described in the following sections.

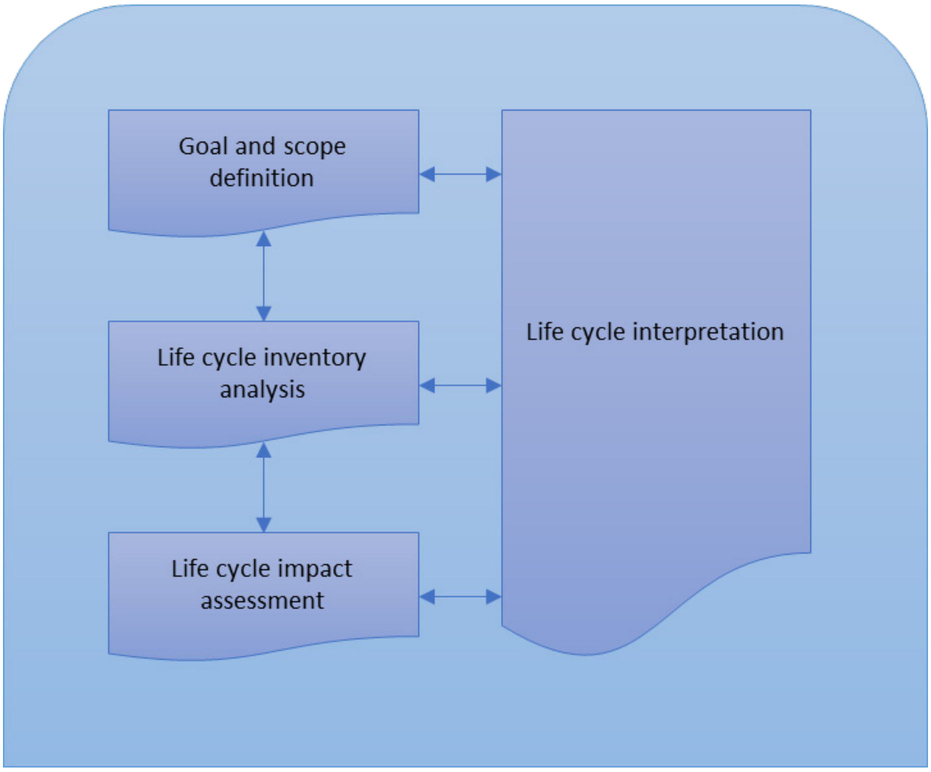

Figure 4. Life cycle assessment framework (based on ISO 2006b)

4.2.2.1. Goal and scope definition

The first step in any LCA study is to clearly define the objective and the scope being consistent with the intended application. As an LCA is an iterative process, the scope might be refined during the study.

On the one hand, the goal of the study must define the intended application, the reasons for carrying out the study and the intended audience. On the other hand, the scope must describe the product system, the functional unit, the system boundaries, the allocation procedures, the LCIA methodology, interpretation to be used, data requirements, assumptions, limitations, data quality requirements, the critical review (if needed), and the format of the report. The most relevant are further explained in the following sub sections.

It's worth to mention that in a comparative study, the systems under comparison must be equivalent in terms of their scope, therefore the systems must share the same functional unit and equivalent methodological considerations.

Function and functional unit

In any LCA study, defining the Functional Unit (FU) is a crucial step, as the function that the product system must perform is specified by the FU. Hence, it must be well defined to serve as the foundation for all LCA comparisons.

System boundary

The system boundaries identify the unit processes of the system that are included in the life cycle inventories (LCI) used to provide data, hence it defines the coverage of the LCA study. System boundaries might be updated from one iteration to another. A cradle-to-grave or cradle-to-gate strategy can be used, depending on the study's goal.

Theoretically, every process that affects the product system under analysis must be considered. However, this would add too much complexity to the LCI stage, so, in practice, only the processes that contribute in a meaningful proportion are included, applying a cut-off criterion. Therefore, every secondary process that makes a smaller contribution is disregarded.

Types of impacts

During this step, impact categories, category indicators and characterization models must be selected according to the goal of the LCA study. For example, the Intergovernmental Panel on Climate Change's (IPCC) provides an impact method, IPCC 2013, with several impact categories, such as Global Warming Potentials (GWPs) over a 100-year time horizon, that include the characterization factors to assess impacts from substance amounts (Stocker et al. 2013)

Sources of data

The data sources depend on the goal and scope of the study, as well as its system boundaries. Typically, it may include a mixture of measured, calculated, or estimated data.

4.2.2.2. Life cycle inventory analysis (LCI)

The LCI phase defines the procedure for collecting the inventory data, their main steps are represented in Figure 5. This phase is the most time-consuming part of an LCA, since data quality and accuracy are essential for producing representative and reliable results. Due to the iterative nature of the LCA framework, the LCI phase is done several times which increases reliability, in particular for those processes having a significant influence on the final outcomes and, therefore, they require the collection of huge amounts of data without compromising its quality.

Furthermore, in this phase, the modeling and methodological approach for solving multifunctionality must be defined, as these decisions directly influence the consequence data collection.

Allocation

Most of the industrial processes are multifunctional, they produce more than a unique product. Therefore, the LCA framework defines an allocation procedure to assign the environmental burdens to the different products.

Whenever possible, allocation must be avoided by subdivision. It consists in dividing the unit process into two or more sub-processes, each one with a single functional unit. Another strategy to avoid allocation is system expansion. This means the addition of functions or processes for making the system comparable, or, on the other hand, the subtraction of functions not needed. The latter is done by defining avoided products or functions, which environmental burdens are subtracted from the assessed process. However, if this substitution triggers market effects, a consequential modelling would be required.

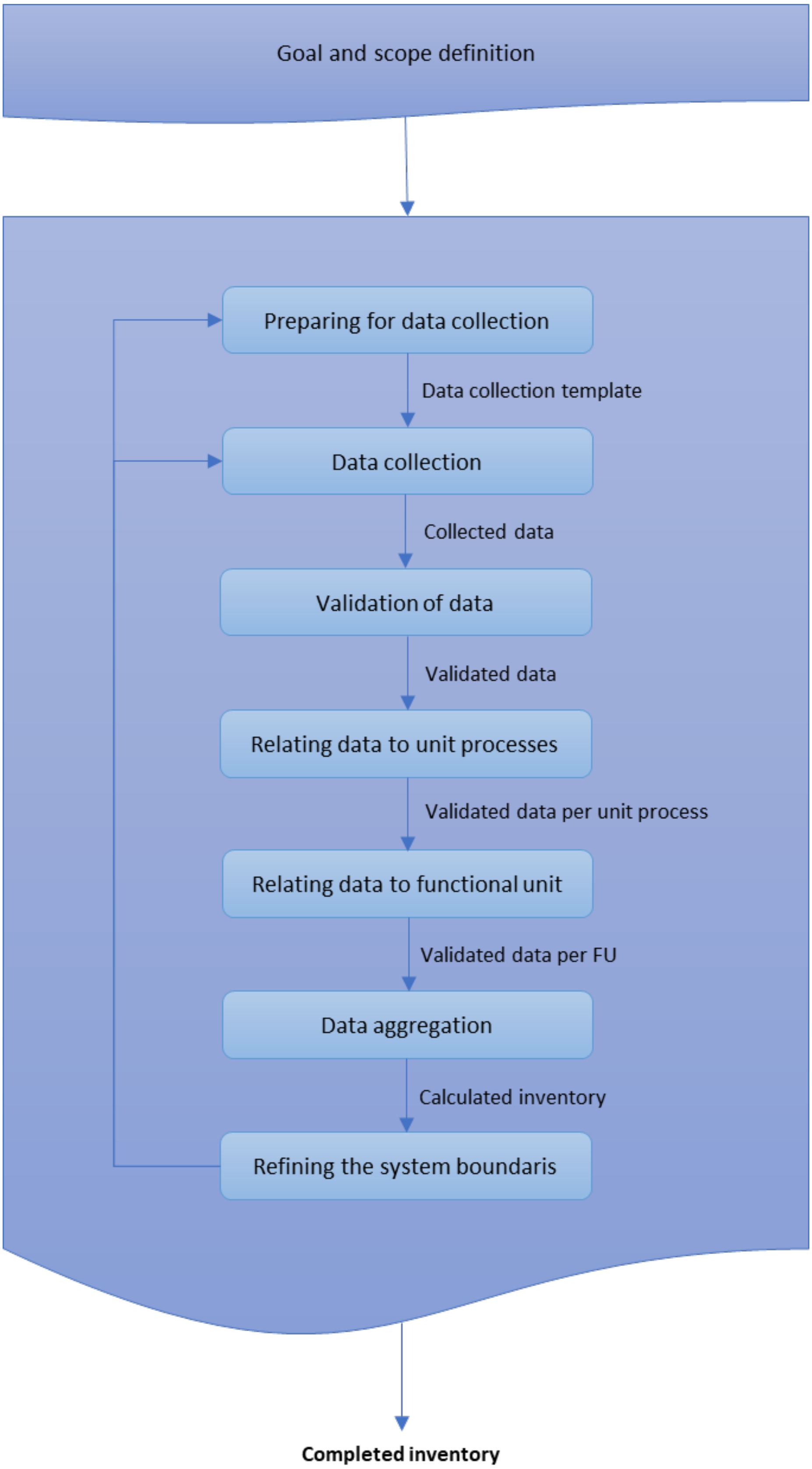

Figure 5. LCI procedure (based on ISO 2006b)

In any other case, allocation should be applied. Allocation attempts to solve the problem of multifunctionality by employing an allocation criterion to divide up a process' inputs and outputs and distribute them according to the process' products. This allocation criterion, according to ISO, should be based on a causal physical relationship between inputs and outputs, or, if this cannot be established, on another relationship, such as their economic worth or energy content.

4.2.2.3. Life cycle impact assessment (LCIA)

In this stage, the environmental flows (inventory data) collected during the LCI phase are aggregated into impact categories. The results are then attributed to environmental damage and analyzed. Furthermore, sensitivity analysis might be used to identify the processes that have a significant impact on the outcomes and for which the next iteration loop may call for more precise inventory data.

Characterization

A LCIA method assigns characterization factors (CF) for each impact category to the environmental flows of the product system, defined as amounts of the reference flow selected for each impact category. For example, for the global warming category the reference flow is CO_2, and all GHG emissions are expressed in CO_2 equivalents (CO_2-eq). This way, applying the characterization factors from the Intergovernmental Panel on Climate Change's (IPCC) 2013 report on Global Warming Potentials (GWPs) over a 100-year time horizon (Stocker et al. 2013) each gram of CO_2 contributes 1g CO_2-eq and each gram of, for instance, CH_4 represents 30.5 g CO_2-eq (Masson-Delmotte et al. 2021).

Normalization

In the LCIA phase, normalization is an optional step. It provides a contribution in relation to a common reference by dividing the characterization results of each impact category by a fixed value. For example, the territorial elementary flows of a nation or a region for a particular year serve as typical normalizing values (e.g., Europe 1995). However, the percentage that the evaluated process would contribute to the average total emissions of that society or process, respectively, might also be determined by using this as a reference process. This facilitates process comparison and identifies the contribution hotspots. Additionally, it makes it simpler to communicate results to people who are unfamiliar with the specifics of LCA methodology. The outcome, on the other hand, is merely a flow of the environment relative to a standard reference and may not always represent the related environmental harm.

Weighting

As normalization, weighting is an optional step during the LCIA phase. In order to reflect the various environmental relevance of the impact categories, it assigns a specific weight to the (often normalized) impact values in each category. However, because the weighting variables are always highly subjective, this must be handled with caution. Therefore, the weighing criteria must be supported and well stated. Finally, it is worth to mention that weighting is necessary to combine many impact categories into a single score.

Impact assessment

During the goal and scope phase, the impact assessment method is chosen. It, not only, should address all relevant impacts for the process under study, but also should produce intelligible results for the potential audience of the study, according to their expertise.

The impact assessment methods are environmental models that link environmental flows of different substances with environmental impacts. These effects are calculated for several categories in order to account for all possible environmental effects. LCIA approaches often employ fate models, with the environmental flows producing an environmental load for a predetermined period (after which the environmental load is reduced by natural processes reaching the background concentration) (J. B. Guinée et al. 2001). This demands an in-depth understanding of how the environment reacts to induced environmental loads. The science base in this regard can be weaker or stronger depending on the impact category evaluated; therefore, the associated uncertainties change. For instance, there is considerable scientific agreement regarding the causes of global warming and how they contribute, as summarized in the IPCC reports (Masson-

Delmotte et al. 2021). However, in other categories, such as eutrophication (emission of micronutrients like nitrates and phosphates to the environment) higher disparity exists. The induced repercussions in this case are more regional and rely on the real environmental load already present at the site, as well as its native flora and fauna. The results achieved for the same process can vary significantly throughout different approaches as a result of these uncertainties.

Several LCIA methods exist. However, a general classification divides them into two categories, midpoint and endpoint level methods (Figure 6). On the one hand, midpoint methods aggregate environmental flows into a set of impact categories. These are distinct from each other and should not be compared to or weighed up together. Due to the numerous categories, they provide an accurate picture of the environmental impacts. However, this frequently makes it difficult to understand the results because there is often no clear-cut conclusions or judgments that can be drawn from them. On the other hand, endpoint methods aggregate the midpoint indicators into damage categories, usually three: damage to human health, damage to ecosystem diversity and damage to resource availability. This gives more comprehensive results; however, it requires weighting which adds another subjective element to the evaluation increasing the uncertainty. Furthermore, some approaches aggregate the three damage categories into one single score. This increases even more simplicity, which is embraced by a certain audience with low knowledge about LCA methodologies, but also increases even more the uncertainty of the results.

As examples, the CML method (J. B. Guinée et al. 2001) is a typical midpoint approach. Meanwhile, a common endpoint method is the Eco-indicator 99 (Goedkoop and Spriensma 2001). There are also hybrid methodologies such as ReCiPe (Huijbregts et al. 2016) which compute midpoint and endpoint indicators.

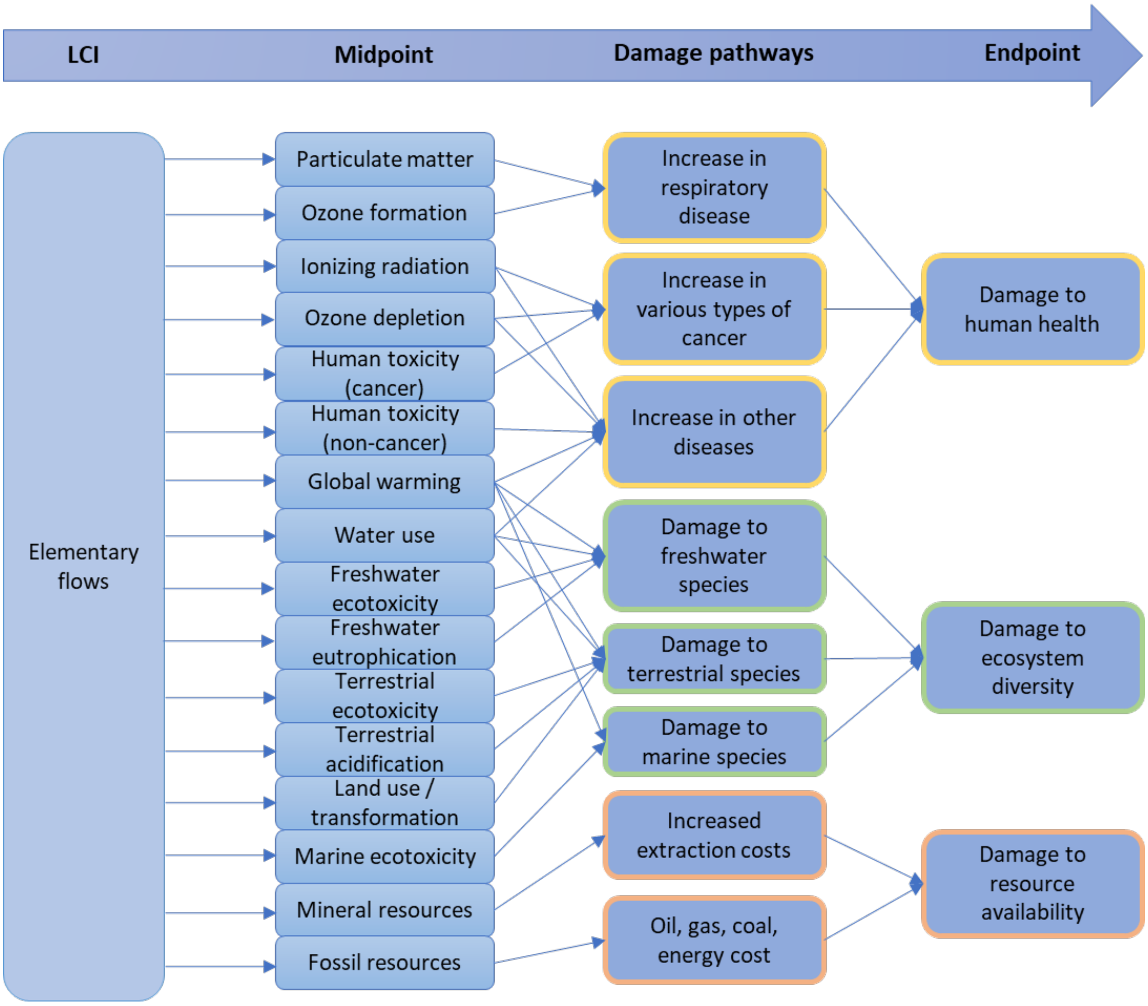

Figure 6. Life Cycle Impact Assessment Methodology

4.2.2.4. Life cycle interpretation

Life cycle interpretation phase comprises several elements: identification of the significant issues based on the results of the LCI and LCIA phases, an evaluation that considers completeness, sensitivity and consistency checks, and, finally, the conclusions, limitations and recommendations of the study. The relationship of the interpretation phase to other LCA phases is shown in Figure 7.

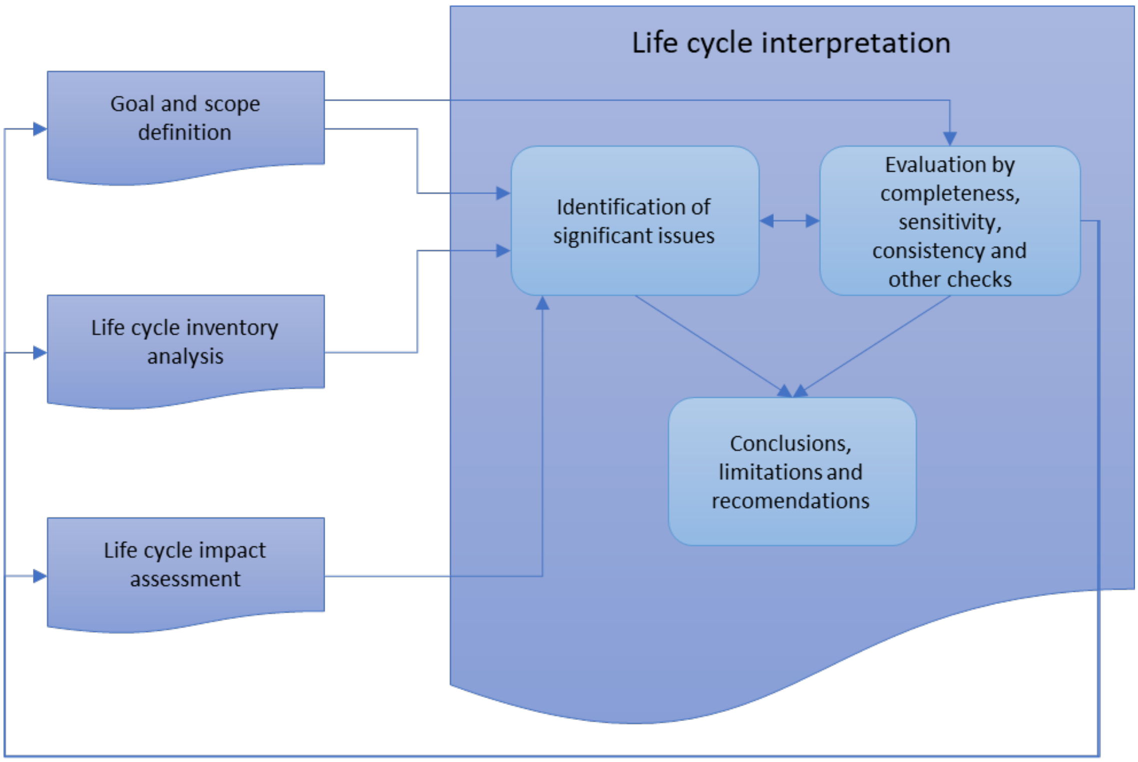

Figure 7. Relationship between other LCA phases and the interpretation phase (based on ISO 2006b)

This phase together with the goal and scope stage of a life cycle assessment frame the study, while the other phases, LCI and LCIA, produce information on the product system under study.

Identification of significant issues

This element's mission is to organize the findings from the LCI or LCIA phases in line with the goal and scope description to identify the key concerns. The main goal is to cover the effects of the techniques employed and assumptions made in the stages that came before it, including allocation guidelines, cut-off choices, impact category selection, category indicators, and model selection.

Evaluation

The goals of the evaluation element are establishing and enhancing confidence, as well as reliability, of the LCA and LCI results; including the significant issues identified in the first element of the life cycle interpretation phase. The evaluation's findings should be presented in a way that any relevant stakeholder can easily grasp the conclusions of the LCA study.

The use of the completeness, sensitivity and consistency checks shall be considered. First, the purpose of the completeness check is to confirm that all pertinent data and information required for the interpretation are complete and available. Then, the goal of the sensitivity check is to evaluate the reliability of the final results and conclusions by identifying how uncertainties in the data, allocation procedures, or outcomes of category indicator calculations affect them. Finally, finding out whether the assumptions, techniques, and data are in line with the goal and scope of the study is the purpose of the consistency check.

Conclusions, limitations and recommendations

The objective of this part of the life cycle interpretation is to draw conclusions, identify limitations and make recommendations for the intended audience of the LCA study. This should be done iteratively with the other elements in the interpretation phase.

4.2.3. Brightway2

Several LCA software tools are currently offered in the market, some of them have a commercial license, such as SimaPro (PRé Sustainability 2022), and others are open-source, such as OpenLCA (GreenDelta 2022). The choose of one tool over another is based on functionality concerns, the availability of databases and datasets, user interface, data quality and management, as well as the modeling principles to create product systems and unit processes. Therefore, it is crucial to understand the significance of these variations and how they may affect LCA outcomes (Silva et al. 2017).

For the development of this thesis, Brightway2 (Mutel 2017) is selected. It is an open-source framework for life cycle assessment (LCA). It is designed to be easy to use, while still being powerful. Brightway2 does not try to replace software packages like SimaPro or OpenLCA, but instead offers possibilities to those who need to break the limits of conventional LCA. Despite of not having a user interface, Brightway2 was selected as main environmental databases are available for it, such as ecoinvent (Wernet et al. 2016); furthermore, its open-source nature eases the process of integrating it into the eco-design tool under development during this thesis work; it also provides fast calculations which is crucial when integrating it within optimization problems; and, finally, no lack of functionalities was identified to fulfill the objective of this thesis.

4.3. Life cycle costing framework (LCC)

4.3.1. Background

As explained in section 1.3.2, LCC is a tool to evaluate the costs associated with a product, process or activity in its whole life cycle, from its design through its production and transport to its end of life. For the development of this thesis, a conventional LCC will be applied, as its methodology is similar to traditional techno-economic analysis (TEA) used in process engineering.

The main limitation of this approach is that end-of-life costs are not considered in the assessment, adopting a cradle-to-gate approach which, therefore, limits the system boundaries adopted in the LCA study, as they must be equivalent to the ones used in the LCC methodology.

4.3.2. LCC approach for industrial processes

Nowadays, there is not a standard applicable to any kind of product when talking about LCC, as it is for LCA. However, there are standards for specific products such as ISO 15686 (ISO 2017), for buildings and ISO 15663 (ISO 2021), for petroleum, petrochemical and natural gas industries.

Therefore, the following approach is based on life cycle thinking methodologies, in particular, conventional LCC and the standardized LCA framework; the existing standards for buildings and petrochemical industries, and, finally, traditional methodologies for cost estimation applied in TEA in the field of process engineering.

As in LCA, the elaboration of a LCC study is an iterative process and requires the collection of huge amounts of data. The main process steps, as applied also within this thesis, are shown in Figure 8 and described in the following sections.

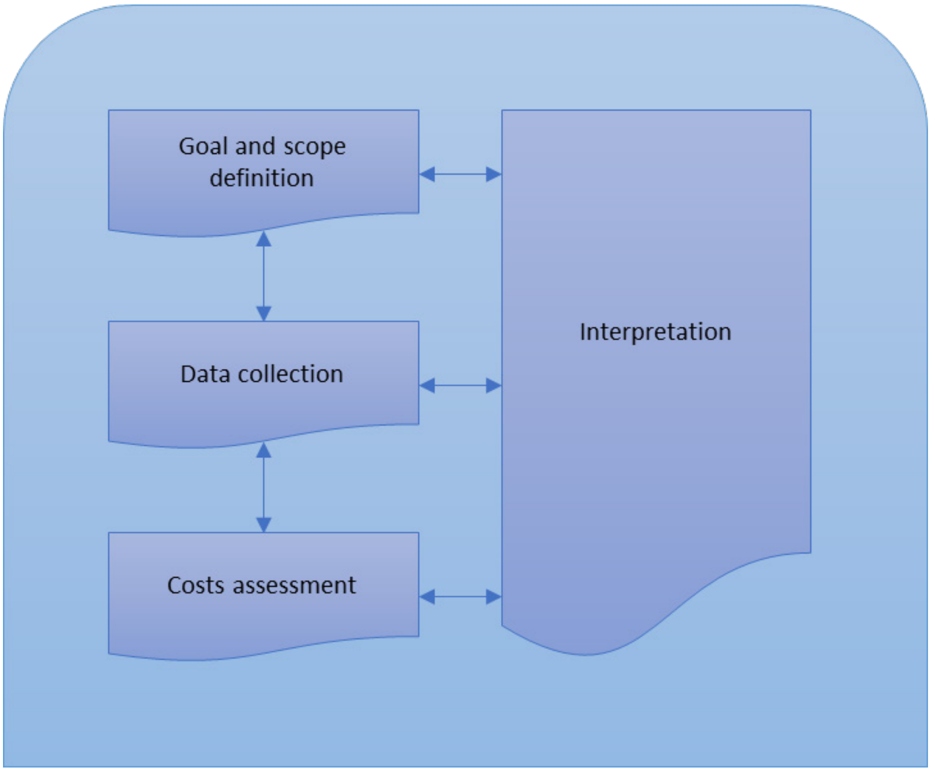

Figure 8. Life cycle costing framework (based on ISO 2006b)

4.3.2.1. Goal and scope definition

The first step in any LCC study is to clearly define the objective and the scope being consistent with the intended application. As an LCC is an iterative process, the scope might be refined during the study.

On the one hand, the goal of the study must define the intended application, the reasons for carrying out the study and the intended audience. On the other hand, the scope must describe the product system, the system boundary, establish economic performance indicators, interpretation to be used, data requirements, assumptions, limitations, data quality requirements, the critical review (if needed), and the format of the report. The most relevant are further explained in the following sub sections.

It's worth to mention that in a comparative study, the systems under comparison must be equivalent in terms of their scope: therefore, the systems must share the same decision criteria, boundaries and equivalent methodological considerations.

System boundary

The system boundary identifies the unit processes of the system that are included in the assessment used to provide data, hence it defines the coverage of the LCC study. Furthermore, it defines the lifetime of the process under study which is crucial to compute relevant economic performance indicators. System boundaries might be updated from one iteration to another. In a conventional LCC, a cradle-to-gate strategy is applied.

Establish economic performance indicators

Economic performance indicators must be established and documented in compliance with asset requirements. These indicators might be used to rank different options and to provide the basis for determining the main cost drivers.

A range of economic performance indicators might be defined, such as, not limited to, the following:

Capital expenditure (CAPEX)

CAPEX are funds used by a company to acquire, upgrade, and replace physical assets such as property, plants, buildings, technology, or equipment.

Operating expenditure (OPEX)

OPEX are expenses during the normal business operations. They include rent, raw materials, utilities, inventory costs, marketing, payroll, insurance, and funds allocated for research and development.

Net Present Value (NPV)

NPV is the difference between the present value of cash inflows and the present value of cash outflows over a period of time. Earnings can be reinvested as soon as they become available and begin to earn a return. Therefore, money made early in the project is worth more than money made later. This is the time value of money, which may be addressed by using a variation of the familiar compound interest formula. This way, the net cash flow in each year is brought to its present value at the start of the project by discounting it at some chosen compound interest rate.

The NPV is calculated using the following formula:

$$NPV = \sum_{n=1}^{n=t} \frac{Net\ cash\ flow\ in\ year\ n}{(1+r)^n} \quad (1)$$

Where r is the discount rate and t the life of the project in years.

The discount rate is chosen to reflect the earning power of money. Usually, it would be equivalent to the current interest rate that the money could earn if invested.

Internal Rate of Return (IRR)

IRR is the discount rate at which the NPV has a value of zero. It measures the maximum rate that the project might pay while maintaining the break even at the end of the project lifetime.

$$\sum_{n=1}^{n=t} \frac{Net\ cash\ flow\ in\ year\ n}{(1+IRR)^n} = 0 \quad (2)$$

Payback period

Payback period is the time required after the start of the project to pay off the initial investment. It is a useful indicator when the project has a short life, or when the capital is available during a short time. Its main limitation is that it does not consider the performance of the project after the payback time.

Levelized cost of production (LCOP)

LCOP is the minimum price at which the product from a process should be sold in order to offset the total costs of production over its lifetime. It is computed solving the following equation:

$$\sum_{n=1}^{n=t} \frac{CF(n, LCOP)}{(1+r)^n} = 0 \quad (3)$$

Where CF is the net cash flow which depends on the year n and the sale price, and r in this case is the expected discount rate by the project stakeholders.

Sources of data

The data sources depend on the goal and scope of the study, as well as its system boundaries. Typically, data sources may provide the following: equipment costs or design parameters (from which costs might be estimated), materials and utilities prices, labor costs, price indexes, interest rate and discount rate, among others.

4.3.2.2. Data collection

The data collection phase defines the procedure for collecting the economic assessment data, its main phases are represented in Figure 9. This phase is crucial since data quality and accuracy are essential for producing representative and reliable results. Due to the iterative nature of the LCC framework, the data collection procedure is done several times which increases reliability, in particular for those processes having a significant influence on the final economic indicator. These are known as cost drivers, identify them is critical to allocate the effort available for the assessment.

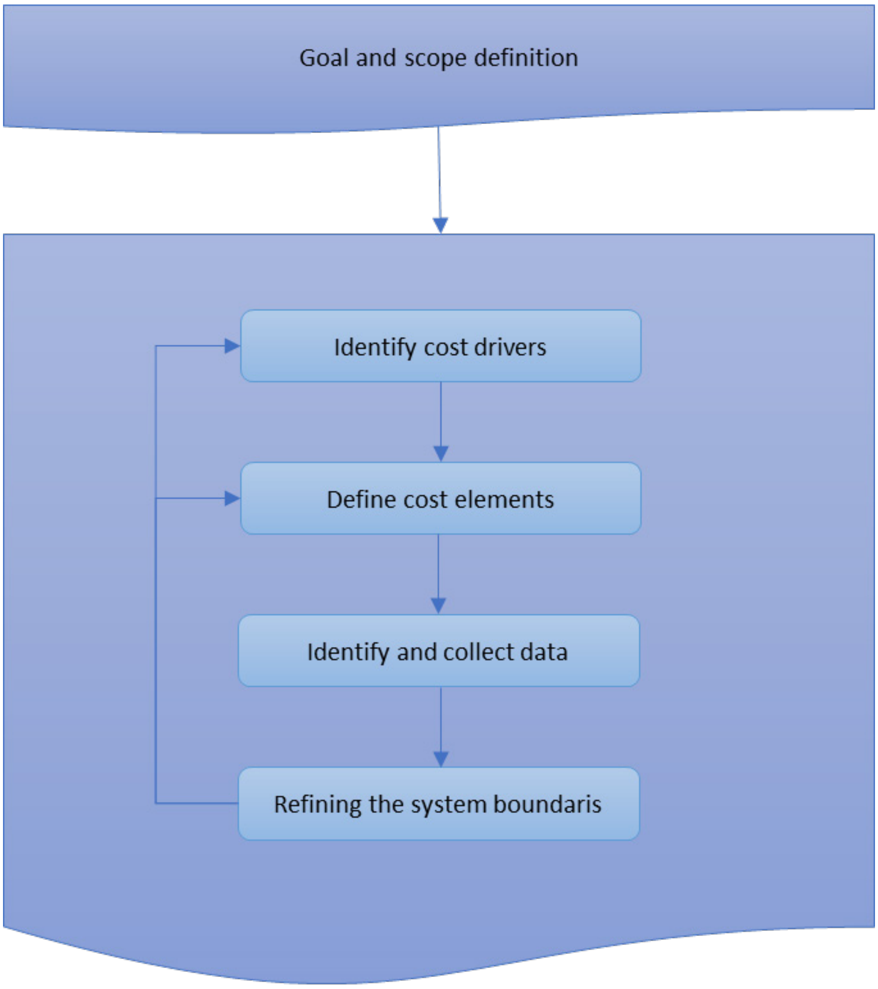

Figure 9. LCC Data collection phase

Once the cost drivers are identified, to determine the minimum number of cost elements required to estimate each cost driver is the next step. However, sometimes it is possible to directly get the cost for a cost driver by comparison with other similar work and, therefore, that particular cost driver does not need to be assessed by its cost elements.

Finally, the data sources identified during the goal and scope phase are used to retrieve the data needed for the calculation of the different cost elements. This is the data collection phase, which is crucial for the success of the LCC study.

Furthermore, in this phase, the modeling and methodological approach for solving multifunctionality must be defined, as these decisions directly influence the consequence data collection.

4.3.2.3. Costs assessment

In this stage, the data collected for the different cost elements is used to compute the CAPEX and the OPEX of the product system (Figure 10). It also populates the cash flow model developed during this phase which produces further economic performance indicators if needed for the assessment. Furthermore, sensitivity analysis might be used to identify the processes that have a significant impact on the outcomes and for which the next iteration loop may call for more precise modelling or input data.

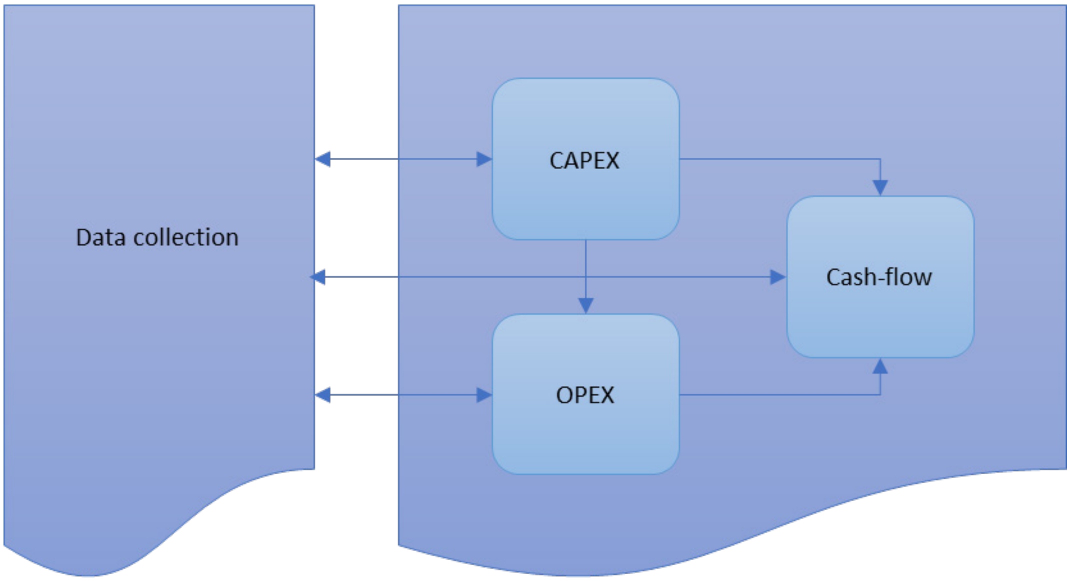

Figure 10. LCC cost assessment phase

The accuracy of a cost assessment relies on the quality and availability of the data and the time spent on the modelling. Only a rough estimate will be needed in the early stages of a project, and it will be justified by the amount of information that has already been gathered. As the project evolves, the different iterations of the LCC study will provide more accurate results.

CAPEX estimation

The CAPEX (Figure 11) of an industrial process is the total cost of designing, constructing, and installing it. It includes:

- The inside battery limits (ISBL) investment, the cost of the plant.

- The outside battery limits (OSBL), the cost associated with the modifications and improvements that need to be done to the infrastructure.
- Design and engineering costs.
- Contingency charges.

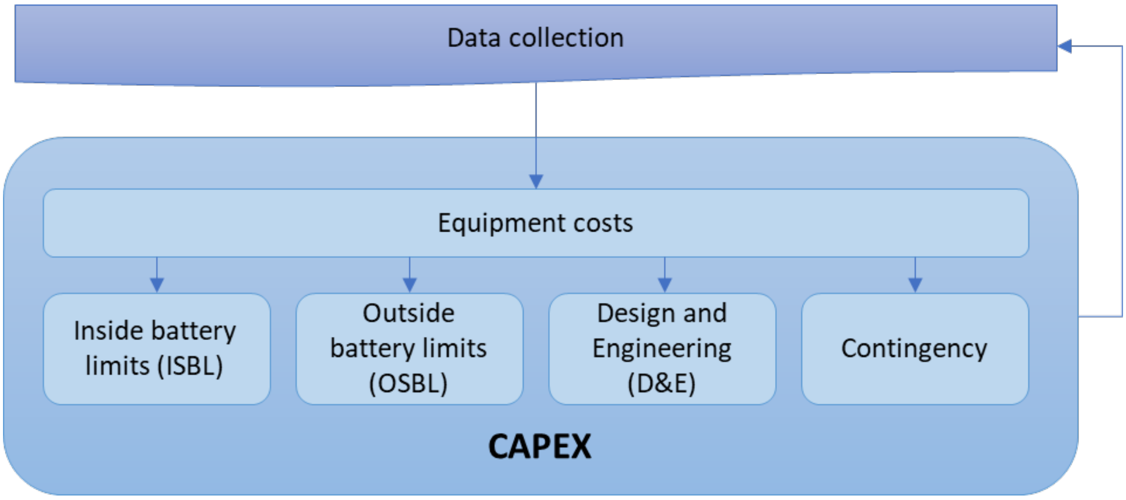

Figure 11. CAPEX estimation

ISBL

The ISBL includes the cost of procuring and installing all the process equipment. On the one hand, it includes the direct field costs:

- All the major process equipment, such as vessels, reactors, columns, furnaces, heat exchangers, coolers, pumps, compressors or turbines, among others; including, if necessary, onsite manufacture and testing.
- Bulk items, such as piping, valves or wiring.
- Civil works such as roads, foundations, piling or buildings.
- Installation labor.

On the other hand, it also includes indirect field costs:

- Construction costs such as construction equipment, transport rental or temporary water and power.
- Field expenses and services.
- Construction insurance.

- Labor benefits and burdens.
- Miscellaneous overhead items such as local taxes, patent fees or legal costs.

Since other project expenses are frequently estimated from ISBL costs, it is crucial to clearly define the ISBL scope during the goal and scope phase. Otherwise, the project economics could be adversely miscalculated.

OSBL

The expenses of the site infrastructure additions necessary to enable the installation of a new process or upgrading an existing one are included in the OSBL investment. It might include, among other things: electric main substations, power generation plants, boilers, water treatment plants, cooling towers, pipelines, air separation plants, instrument air lines, loading facilities, warehouses, laboratories, offices, maintenance facilities and emergency services. OSBL costs are typically estimated as a proportion of ISBL in the early stages of a project.

Design and Engineering

This investment includes the cost of detailed design and other engineering services required to carry out the project.

Contingency

Contingency charges are extra costs added into the project budget to allow for variation from the initial cost estimate. Furthermore, it also covers changes in project scope or prices, currency fluctuations, labor or subcontracting problems and other unexpected issues.

OPEX estimation

The OPEX investment of an industrial process is divided into fixed costs and variable costs of production (Figure 12).

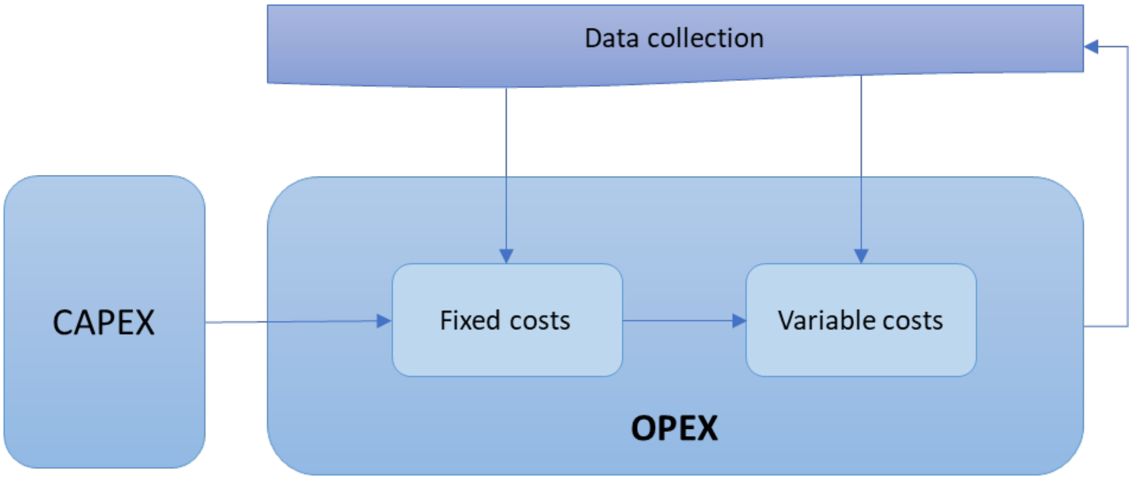

Figure 12. OPEX estimation

Fixed costs of production

Fixed costs associated with production are expenses that are incurred independently of the plant output or operation rate. Therefore, they are not decreased if the plant reduces its output. Fixed costs include:

- Operating labor and supervision.
- Direct salary overhead (employees' health insurance and other benefits).
- Maintenance costs.
- Property taxes and insurance.
- Rent of land.
- General plant overhead (research and development, information technology or finance).
- Environmental charges.
- Fees and royalties.
- Capital charges, such as interest payments and depreciation.
- Sales and marketing costs.

Usually, fixed costs are estimated as a fraction of CAPEX estimations and must not be neglected, as they have a significant impact on project economic performance.

Variable costs of production

Variable costs of production are costs that are proportional to the plant output or operation rate, including: raw materials, utilities, consumables, effluent disposal and packaging and shipping.

Price data is key in order to assess a reliable estimation of the variable costs, as they are calculated multiplying the annual consumption (of raw materials or utilities) by the price. On the other hand, consumables and disposal costs are usually estimated as a fraction of fixed costs such maintenance cost.

Cash Flow estimation

The cash flow estimation provides aggregate data regarding all cash inflows a project receives from its ongoing operations and investment sources. It also includes all cash outflows that pay for plant activities and investments during a given period. As a result of a cash flow model (Figure 13), a cash flow statement is obtained.

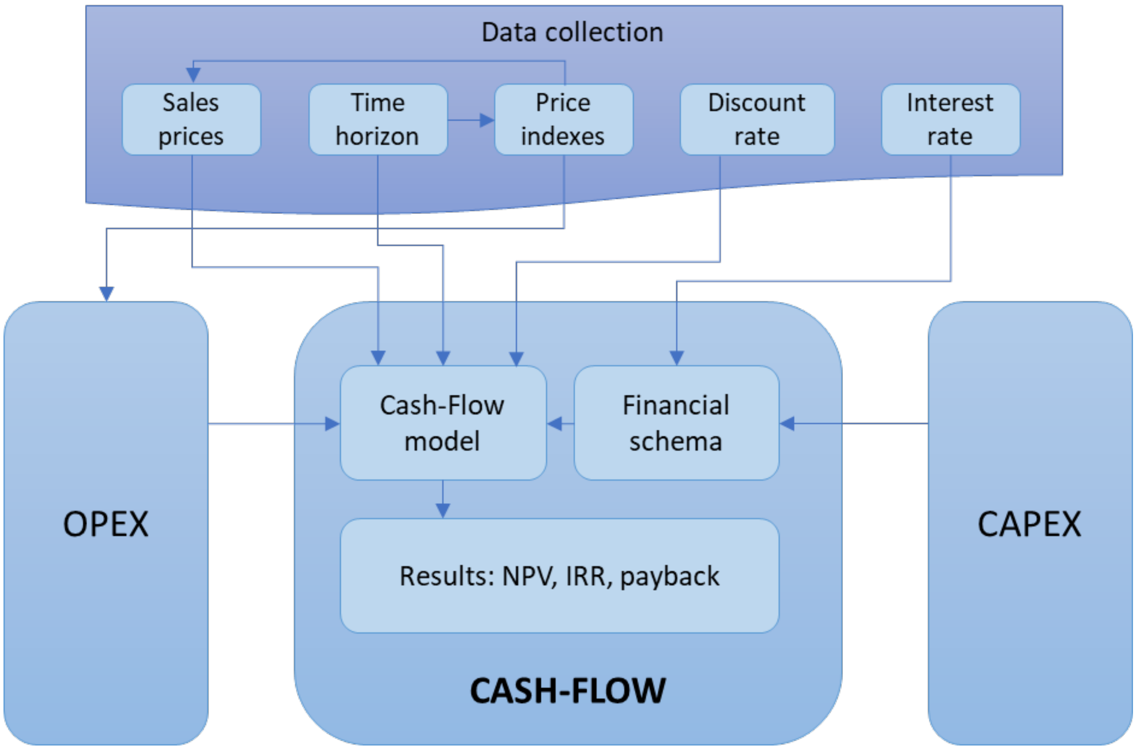

Figure 13. Cash flow estimation

In order to create the cash flow statement, the CAPEX estimation is used as initial investment. Furthermore, a financial scheme must be determined defining the amount of the initial investment that will be covered by own resources. The rest, hence, will be covered by a loan.

On the one hand, OPEX estimation is used to get the annual cash outflows during the project lifetime. On the other hand, to compute the cash inflows a process revenue must be estimated. It is the income earned from sales of main products and by-products of the industrial process. Finally, the gross profit is computed subtracting the outflows from the inflows, then the net profit is obtained subtracting the taxes. Moreover, another economic performance indicators might be inferred from the cash flow statement such as the EBITDA (Earnings before interest, taxes and depreciation), EBIT (Earnings before interest and taxes), EBT (Earnings before taxes) and EAT (Earnings after taxes or net profit). The process to get the annual cash flow is shown in Figure 14.

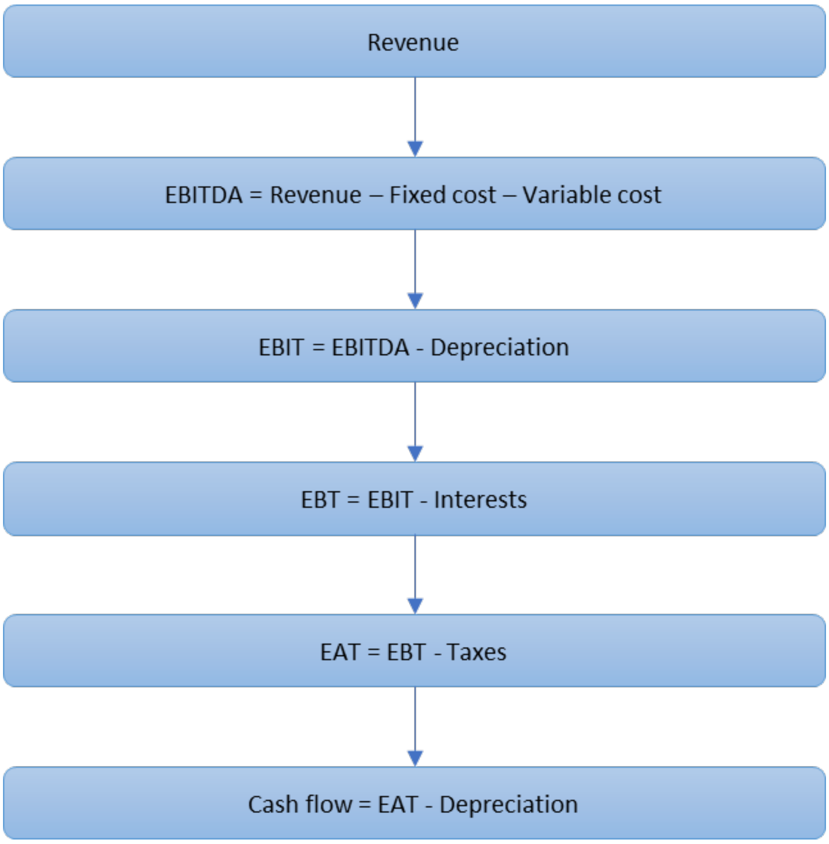

Figure 14. Cash flow computation

Finally, having the cash flows of the project and a discount rate, equations 1 and 2 might be used to calculate the NPV and the IRR. While payback period, is the time when the aggregated cash flow turns positive during the project lifetime.

Price fluctuations

Since the costs of capital assets, materials and labor are subject to inflation, this must be considered in a cash flow modelling phase as it is done during the whole lifespan of the project. To get prices up to date price indexes must be collected during the data collection phase, then the following formula might be applied:

$$Cost_{year\ 1} = Cost_{year\ 0} \frac{Price\ index_{year\ 1}}{Price\ index_{year\ 0}} \quad (4)$$

Furthermore, when estimating future prices these indexes need to be forecasted.

4.3.2.4. Interpretation

The interpretation phase comprises the following elements: identification of the significant issues based on the results of the previous phases, an evaluation that consider, at least, sensitivity checks, and, finally, the conclusions, limitations and recommendations of the study. The relationship of the interpretation phase to other LCC phases is shown in Figure 15.

This phase together with the goal and scope stage of a life cycle assessment frame the study, while the other phases produce information on the product system under study.

The interpretation steps for the LCC study are aligned to those presented in section 3.2.2.4.

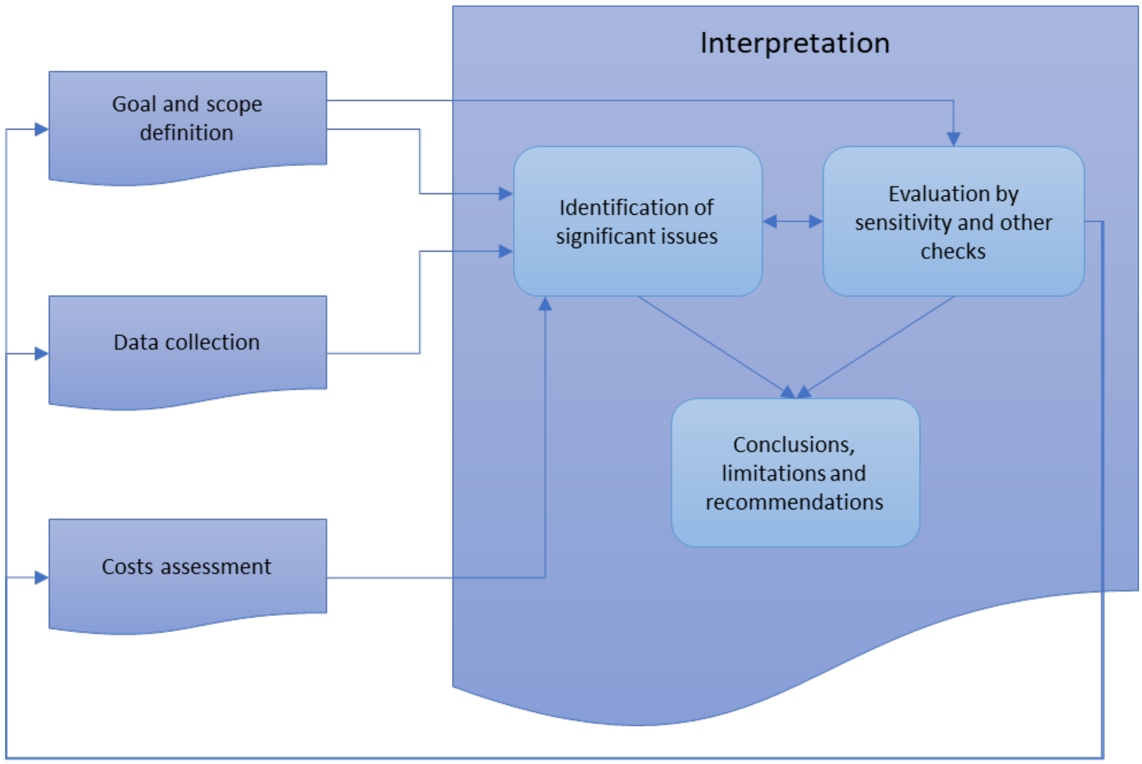

Figure 15. Interpretation phase in a LCC study (based on ISO 2006b)

4.3.3. New Python module

There are numerous cost estimation tools for process engineering accessible, such as Aspen Process Economic Analyzer, APEA (AspenTech 2022b) that provides CAPEX and OPEX estimates. Furthermore, the use of Excel spreadsheets is widely standardized in the industry. However, the first is under a commercial license and does not provide a flexible cash flow modelling; and the last is tedious when it comes to automation and integration with other tools. Therefore, for the development of this thesis a new cost estimation tool has been developed from scratch using Python.

Python is a high-level, general-purpose programming language, dynamically-typed and garbage-collected (Python Software Foundation 2022). It supports multiple programming paradigms, such as structured, object-oriented and functional programming, which makes it flexible. Furthermore, it emphasizes on code readability and easiness. Finally, there are several available libraries for data processing, data analysis, scientific computing and data visualization; and one of the tools selected for the development of this work, Brightway2, is already written in Python.

4.4. Multi-objective optimization framework

4.4.1. Background

Most optimization problems in the real world are multi-objective in nature, therefore solving them requires satisfying two or more conflicting functions. These problems are referred to as multi-objective optimization problems (MOOPs). The optimum in this kind of problems is not a single solution, but a set of solutions known as the Pareto optimal front. Any element of this set is not better than the others for all the objectives. Therefore, the Pareto front might be used by decision makers to choose the best trade-off solution according to their preferences.

The general multi-objective optimization problem may be expressed as follows:

$$Minimize: \quad F(x) = \{f_1(x), f_2(x), \dots, f_m(x)\}$$

$$Subject\ to: \quad x = [x_1, x_2, \dots, x_n] \in X$$

$$l_i \leq x_i \leq u_i \quad i = 1,2,\dots,n$$

$$g_i(x) \leq 0 \quad i = 1,2,\dots,p$$

$$h_i(x) = 0 \quad i = 1,2,\dots,q$$

Where F(x) is the m-dimensional objective vector, x is the n-dimensional decision vector and X is the n-dimensional decision space. Then, g_i represents the i-th inequality constraints and h_i represents the i-th equality constraints. p and q are the numbers of inequality and equality constraints, respectively. Finally, l_i and u_i represent the lower and upper limits of the i-th decision variable, respectively.

It is worth to mention the following definitions:

- **Feasible solution:** A candidate solution x in X that satisfies the constraints.
- **Pareto dominance:** Given two feasible solutions x and x', the solution x dominates the other solution x' if $f_i(x) \leq f_i(x')$ for all I functions in F, and there is at least one I such that $f_i(x) < f_i(x')$.

- **Pareto optimal solution:** Given a feasible solution x, if and only if x is not dominated by any other feasible solution, x is a Pareto optimal solution.
- **Pareto front:** A set consisting of all objective vectors corresponding to the Pareto optimal solutions. An illustrative two-dimensional Pareto front is shown in Figure 16.

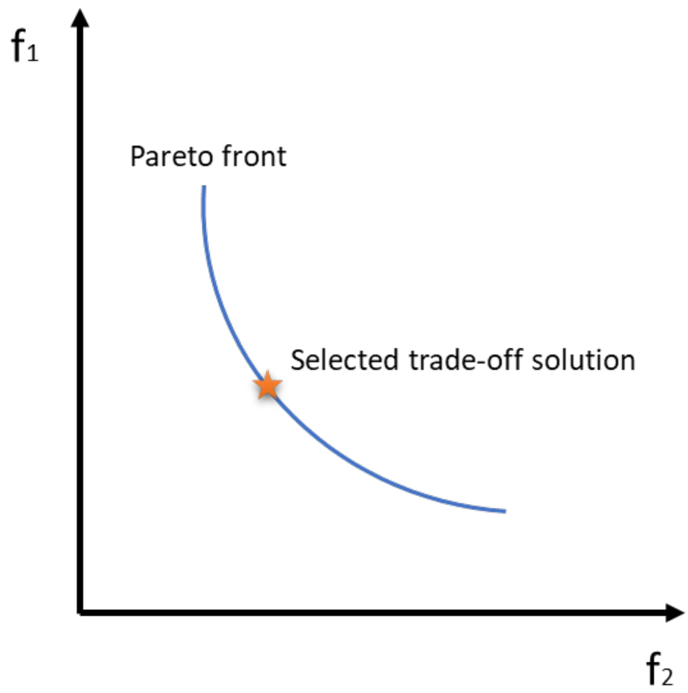

Figure 16. Pareto front for a two-dimensional optimization problem.

4.4.2. Multi-objective optimization approach

The main steps to tackle a multi-objective optimization problem are shown in Figure 17. It is an iterative process, which is followed until a reliable optimal solution is obtained.

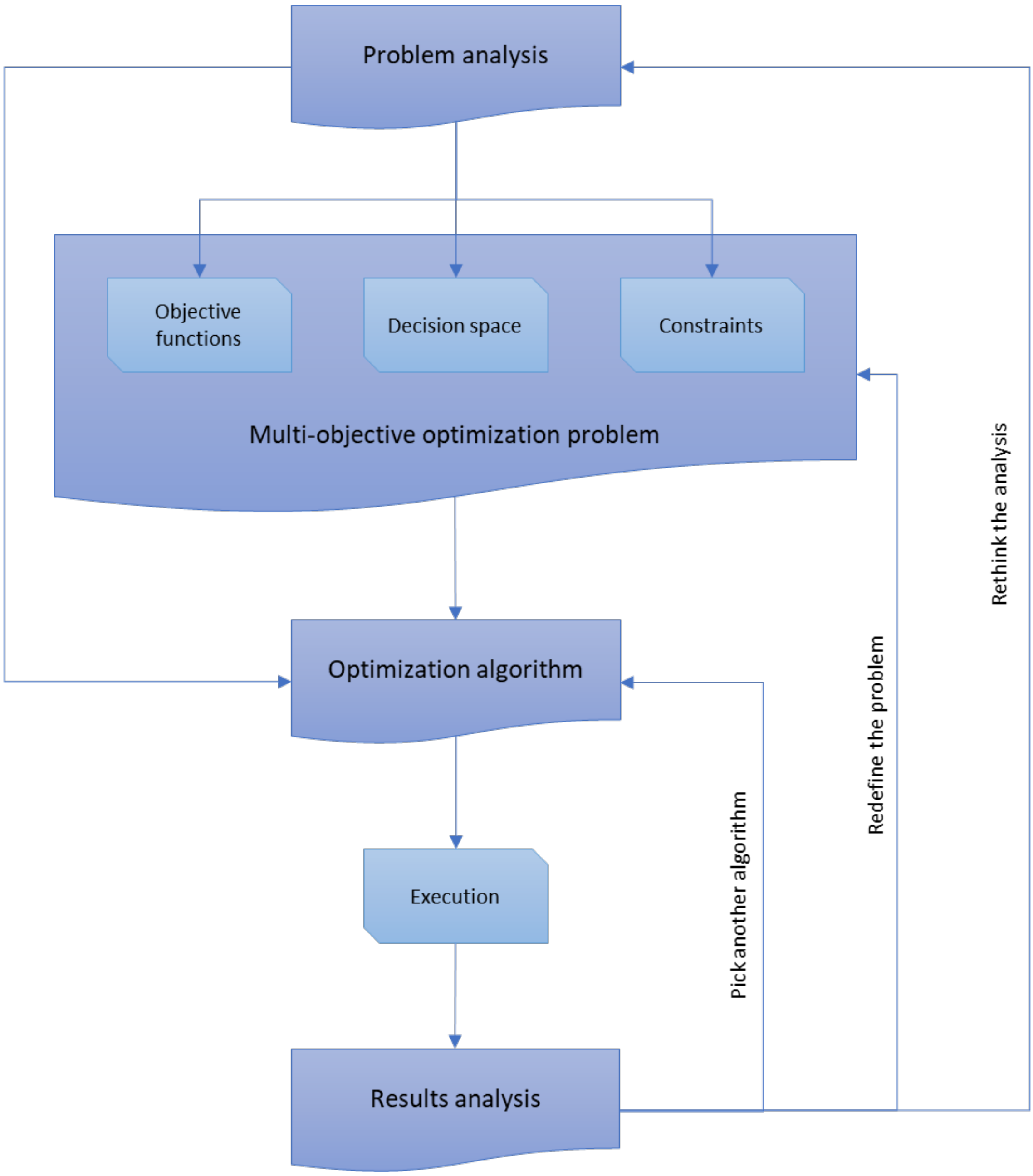

Figure 17. Multi-objective optimization approach.

4.4.2.1. Problem analysis

The first step is to have a good understanding of the problem to be optimized. For that, it is needed to:

- Understand the optimization objectives. It means to know the quantities that will be maximized or minimized. These must be independent and conflicting, otherwise a single-optimization problem might be enough.

- Define the decision space by identifying the decision variables and their bounds. Furthermore, the decision variables must be classified between discrete and continuous.
- Know the functions that relate the decision variables' domain with the objective's codomain.
- Perform sensitivity analysis is highly recommended to understand which decision variables are key in the optimization problem and which are their bounds. This way, variables found to be insensitive are filtered out, as well as the decision space is constrained into the bounds that really have an impact in the objectives. During this step, perform the sensitivity analysis on one objective at a time might give better insights.
- Identify the problem constraints and classify them into inequalities and equalities.

4.4.2.2. Formulate multi-objective optimization problem

Once a good understanding of the problem to solve is reached, the multi-objective optimization problem may be correctly formulated.

4.4.2.3. Choose optimization algorithm

The selection of an appropriate multi-objective optimization algorithm is a challenging process, since sometimes it is not possible to get the holistic viewpoint of how different algorithms will perform solving a specific problem. However, for solving multi-objective problems meta-heuristic algorithms are preferred (Panwar, Tripathi, and Jha 2019; Mirghaderi and Modiri 2021), as they perform better for complex and wide scope problems.

Literature review

During this phase, carrying out a literature review of similar optimization problems might help to have a qualitative view of which specific algorithm could be used. Also, several algorithms could be chosen and postpone the final decision in further iterations.

4.4.2.4. Results analysis

Once the multi-objective optimization problem is executed and solved, it is not common to have a good solution in the first iteration. First, the objectives must be analyzed, since unless having done a good problem analysis step, it might turn out that some objectives are non-conflicting and, therefore, the problem needs to be reformulated. Furthermore, checking the Pareto front decision vectors might help to better understand the decision space and fine tune the variables that really have an impact in the results and their bounds. Therefore, further sensitivity analysis might be performed and, hence, the problem must be reformulated.

During this step, the performance of the chosen algorithm or algorithms must be analyzed. When several algorithms have been used, generational distance and spread metrics in the Pareto fronts might be used to identify which algorithm perform better. Such metrics are included in the commonly used hypervolume indicator (Bradstreet 2011).

Once a reliable solution is reached during the iterative process, qualitative methods are applied to get conclusions from the results. Visualization techniques are widely used to analyze the Pareto front and the decision space, these way stakeholders might select one trade-off solution for further analysis and understanding the characteristics of the problem.

4.4.3. Pygmo

Knowing that the LCA and LCC tools selected for the development of this thesis are written in Python, an optimization library as well written in Python may ease the development of the eco-design tool. Therefore, pygmo (Biscani and Izzo 2020) was selected. It is a scientific Python library for massively parallel optimization. It is built around the idea of providing a unified interface to optimization algorithms and problems, and to make their deployment in massively parallel environments easy. pygmo can be used to solve constrained, unconstrained, single objective, multiple objective, continuous and integer optimization problems, stochastic and deterministic problems, as well as to perform research on novel algorithms and paradigms, and easily compare them to state-of-the-art implementations of established ones.

It was chosen over another optimization libraries, such as scipy (Virtanen et al. 2020), for two main reasons: pygmo offers a wide range of optimization algorithms compared to other libraries and its object-oriented design providing interfaces for both algorithms and optimization problems eases the process of inherit from them and create custom classes in our eco-design tool. Furthermore, pygmo has wrapper classes that allows using scipy algorithms as well.

5. ECO-DESIGN FRAMEWORK FOR INDUSTRIAL PROCESSES

5.1. Background

As stated in Section 1, there are several life cycle approaches and tools to assess sustainability of processes that are applicable in the industrial sector. Furthermore, companies, governments and consumers are demanding a more sustainable production and consumption, even through policies that promote a more sustainable economy.

While having standards and state-of-the-art methods to assess environmental and economic performance in the industry (Section 4), there is not a clear integrated and interoperable methodology for the industrial sector as concluded in the state-of-the-art review. This means that often environmental impacts and costs are assessed separately with different system boundaries. As a result, the decision makers can hardly compare both assessments and draw relevant conclusions. Furthermore, it might happen that data sources are not consistent with each other. For example, the environmental assessment might rely on literature data while the economic assessment might use calculated data from a simulation. This way, comparison is even less reliable between both results. Hence, any multiple criteria analysis carried out by decision makers using these results would not give relevant conclusions or produce misleading findings based on an heterogenous set of assumptions.

This problem is worsened by the fact that during the development of new innovative processes, there are no industrial data that can support any assessment, which gives rise to numerous trial-and-error phases during technology upscaling, exorbitantly increasing time-to-market and costs, while achieving solutions that might not be optimized or, even, feasible in sustainable terms.

Thus, one of the main objectives of this this thesis is to formulate an eco-design framework for industrial processes that overcomes the presented problems unifying the existing standards and state-of-the-art methods described in Section 4. This new framework developed during the PhD work is presented in this section.

5.2. Eco-design framework approach for industrial processes

The proposed framework approach is based on life cycle thinking methodologies and their existing standards, as well as adopting the process simulation and multi-objective optimization frameworks presented above, with the main objective of developing an integrated methodology for the eco-design of industrial processes joining process simulation, LCA, LCC and mathematical optimization. The main steps of this framework are shown in Figure 18.

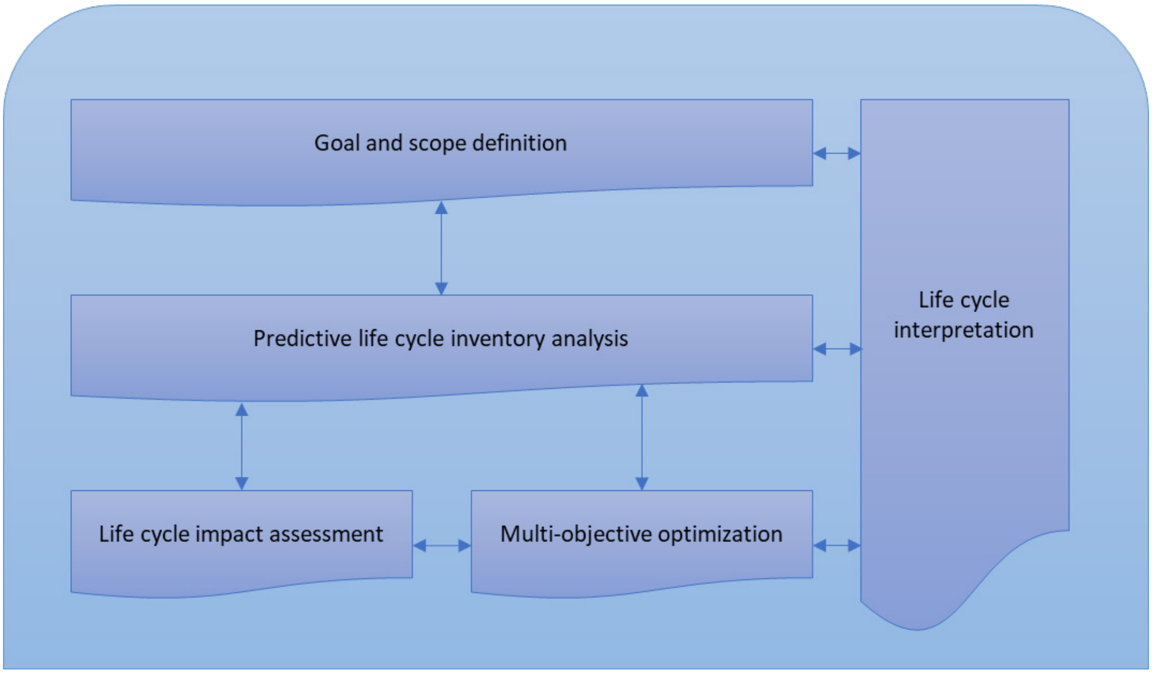

Figure 18. Eco-design framework for industrial processes

5.2.1. Goal and scope definition

The first step in any life cycle study is to clearly define the objective and the scope being consistent with the intended application. As this approach is an iterative process, the scope might be refined during the study.

In this framework, the intended application is to elaborate an industrial process design that minimizes the environmental impacts and costs by considering its life cycle without compromising the technical constraints of the technology. Therefore, within this framework all studies share a common goal that is refined considering the application details, the reasons for carrying out the study and the intended audience. For example, it could be applied for optimizing the scale-up of a new technology or for optimizing the operation of an existing plant in real time through its predictive model or digital twin.

On the other hand, the scope must describe the product system, the functional unit, the system boundaries, the allocation procedures, the LCIA methodology, the LCC performance indicators, define the optimization objectives and decision space, identify the problem constraints, interpretation to be used, data requirements, assumptions, limitations, data quality requirements, the critical review (if needed), and the format of the report.

5.2.1.1. Product system

The product system is represented by the foreground system and the background system. On the one hand, the foreground system is the industrial process itself which within this framework shall be modelled using physicochemical relationships and predictive models generating a process simulation diagram as explained in Section 4.1.2.1. On the other hand, the background system represents all the processes and activities that are necessary to support the foreground system, but that are not directly included in it. This includes the extraction and production of raw materials, the production of energy and any other relevant inputs, and the transportation and waste management systems that support the foreground system. Therefore, all these requirements in the background system should be identified to make the best choice of environmental background databases and cost references that will support the study.

5.2.1.2. Function and functional unit

Defining the Functional Unit (FU) is a crucial step, as the function that the product system must perform is specified by it. Hence, it must be well defined to serve as the foundation for the LCA and the LCC models. Furthermore, it is highly recommended that the FU is also used to compute at least one economic indicator in the LCC model such as the levelized cost of production (ea. €/FU).

5.2.1.3. System boundary

The system boundaries identify the unit processes of the system that are included in the life cycle inventory (LCI) used to provide data, hence it defines the coverage of the study. Since the goal in this framework is to carry out a sustainability-based optimization of the industrial process, a cradle-to-gate strategy is enough. For instance, use phase decisions does not affect the process operation performance. Furthermore, this boundary is consistent with the conventional LCC approach illustrated in Section 4.3.2.

The decision to employ a cradle-to-gate strategy for the initial optimization holds its merits, especially in the context of design phase decision-making. However, a comprehensive assessment of sustainability should not be limited to just this scope. For example, consider the case of fuel production. When analyzing biofuels in comparison to fossil fuels, a cradle-to-gate (or well-to-tank) assessment might show biofuels having a higher environmental footprint. But, when the analysis is extended to a cradle-to-grave (or well-to-wheel) perspective, accounting for combustion and end-of-life processes, fossil fuels often exhibit a significantly larger impact. This underscores the importance of expanding system boundaries post optimization. To ensure a holistic view of environmental and economic impacts, it is recommended that, following the process design optimization using the identified decision variables, a secondary study using a cradle-to-grave approach be conducted.

5.2.1.4. Types of impacts and objectives

During this step, impact categories, category indicators and characterization models must be selected according to the goal of the LCA study. Furthermore, the economic performance indicators are also stated along with the LCC modelling approach. From these economic and environmental impacts, those more relevant according to the goal of the study must be selected as objectives for the optimization problem.

5.2.1.5. Decision space

The decision variables must be identified during this step. On the one hand, relevant design variables that affects the process simulation are selected. Then, topological variables, such as the selection of one technology or raw material over another, are stated. In further iterations, the decision space is refined thanks to the preliminary results and the application of sensitivity analysis.

5.2.1.6. Problem constraints

The technical constraints are defined inside the process simulation and, therefore, they are satisfied as the model would not converge in any other case. However, environmental and economic constraints need to be identified with the relevant stakeholders. Some examples of them are stakeholders not interested in any solution with a negative NPV, or the process under development must be net-zero in terms of carbon accounting. Once they are identified, constraints are classified into inequalities and equalities.

5.2.1.7. Sources of data

The data sources are influenced by the goal and scope of the study, as well as its system boundaries. Typically, they encompass a blend of measured, calculated, or estimated data. It is pivotal to emphasize the role of data quality at this juncture. Adhering to existing life cycle thinking standards, data quality assessment should be performed to ensure reliability, consistency, and relevance. Criteria such as time-related coverage, geographical coverage, technological relevance, precision, completeness, and methodological appropriateness and consistency should be evaluated. Data sources that align with these criteria help in reducing uncertainties and ensuring robust results. Following the quality assessment, the simulation results, which include material and energy balances, together with background databases or other state-of-the-art references will serve to populate both the LCA and LCC models.

5.2.2. Predictive life cycle inventory analysis (P-LCI)

The P-LCI phase defines the procedure for collecting the inventory data, their main steps are represented in Figure 19. This phase is the most time-consuming part of an eco-design study since data quality and accuracy are essential for producing representative and reliable results. Due to the iterative nature of the framework, the P-LCI phase is performed several times, which increases reliability.

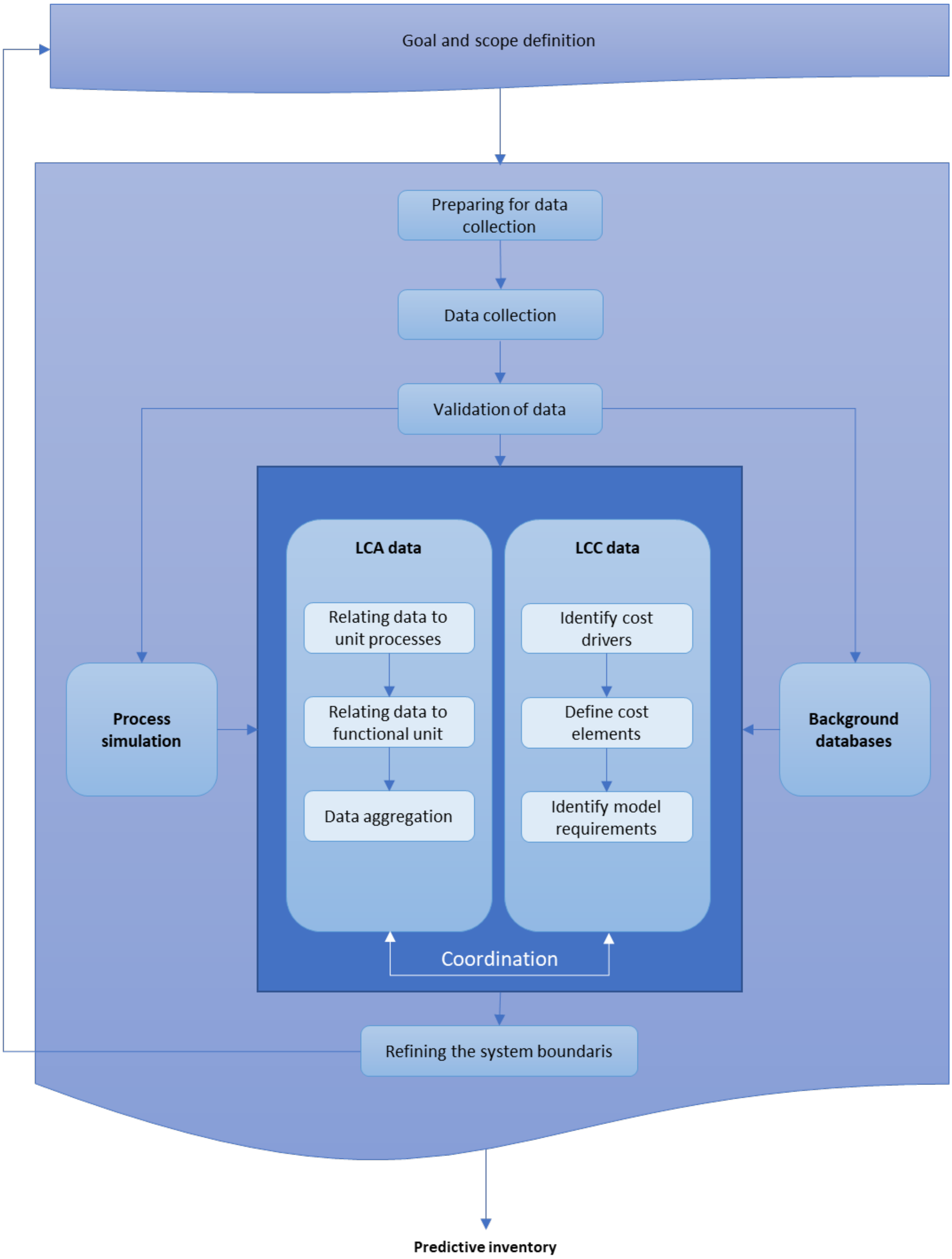

Figure 19. Predictive life cycle inventory in the eco-design framework for industrial processes

In this phase, the modeling and methodological approach for each life cycle study in the framework must be defined, as these decisions consequently influence data collection in a direct manner.

In contrast with the inventory analysis phases in conventional LCA and LCC studies, at the end of this phase the result is a parametrized and predictive inventory connected to the simulated process. Therefore, if any input is modified in the simulation the inventory will reflect the changes automatically. This behavior is crucial to embed the inventory in an optimization problem.

For the detailed data collection, the steps from each life cycle pillar are followed: LCA and LCC; see sections 4.2.2.2, 4.3.2.2, respectively. However, the most important step is the coordination of the data collection procedures. To ensure this coordination during this stage, the following must be stated:

- Identify simulated data that will populate the LCA and LCC models. This way the rest of needed inputs shall be collected from other data sources such as background databases that follow the abovementioned data quality criteria.
- Identify the origin of the optimization objectives.
- Define how to add the decision variables to the simulation, with special care on how to handle topological variables. These might be tackled by design specs or even by two (or more) completely different simulation models.
- Introduce technical constraints in the simulation and define further needed constraints and the data needed to model them.

5.2.2.1. Process simulation model

Since the goal and scope definition and the predictive inventory phases are built around the process simulation model, the LCA model, the LCC model and the MOO problem. At this point, there is consistent data for producing a simulation model that provides the needed inputs for the LCA and LCC models, reproducing at the same time predictive results for different design configurations which allows the integration of mathematical optimization without losing convergence in the decision space. The main stages of this subphase are represented in Figure 20.

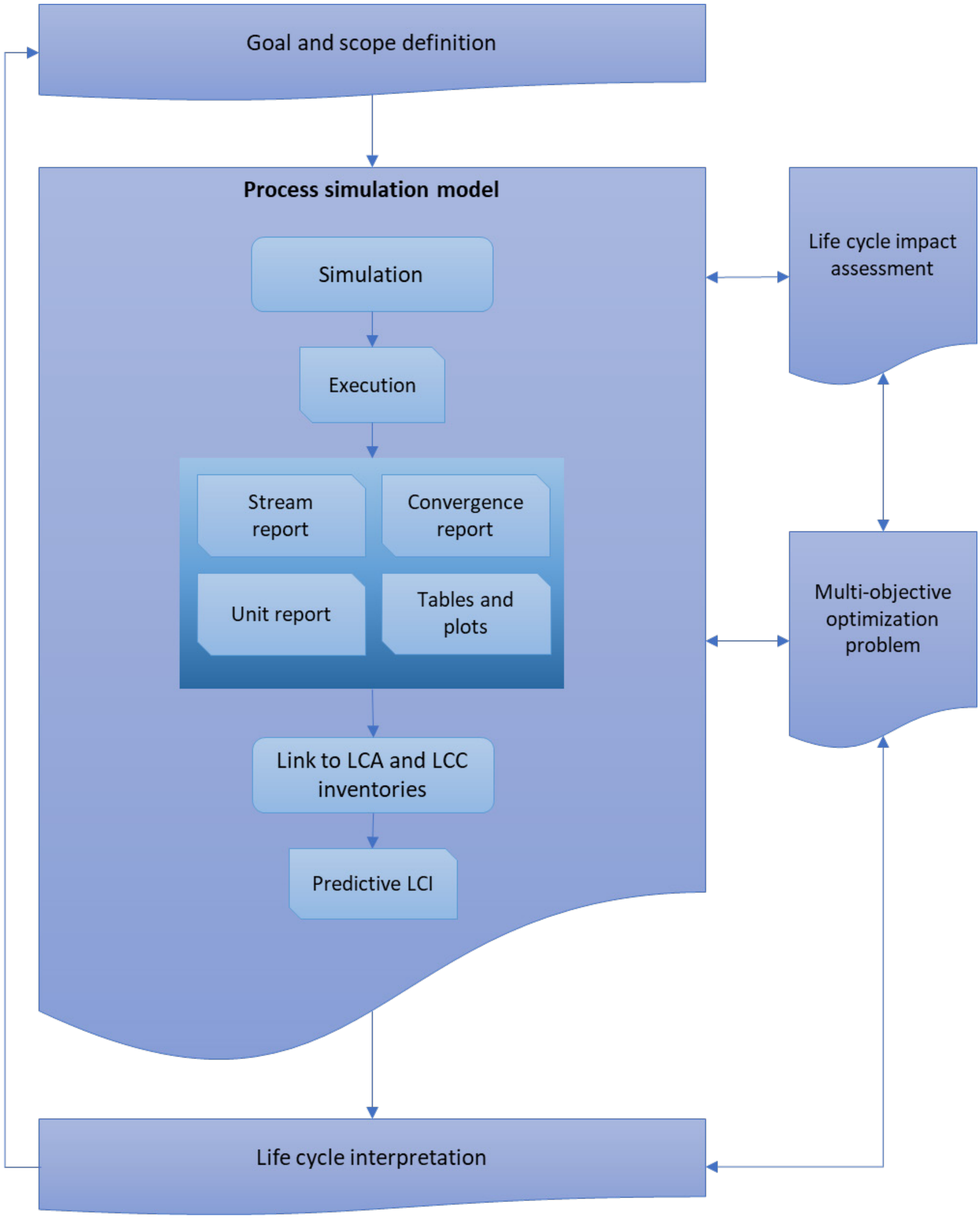

Figure 20. Process simulation model in the eco-design framework for industrial processes

Producing a reliable simulation model is an iterative process in which the collected data define the components, the thermodynamic model, the process flowsheet, the input streams, the system units and the computational strategy. This loop is maintained until reliable results that converge in the identified decision space for the optimization problem are achieved. If this condition is not satisfied, the problem must be reanalyzed adopting strategies such as modifying the decision space or making the simulation model more flexible by getting rid of complex models that cannot adapt themselves to changes in the design variables (distillation columns are a good example of this). One strategy to maintain these rigid models is to generate several simulations, each one of them performing well in a subdomain of the decision space. However, it dramatically increases the complexity of the project.

Note that the simulation model is connected to the LCIA of environmental and economic indicators, and the MOO problem in Figure 20. This is because in the eco-design framework for industrial processes the simulation acts as source of inventory data for them. This way in each generation of the optimization problem and for each individual of the population the predictive inventory is created solving the simulation. Then this data is used to solve the problem using the LCA and LCC models which along with the simulation provide the objectives for the optimization process.

5.2.3. Life cycle impact assessment (LCIA)

In this stage, the predictive inventory data collected during the previous phase is used by the LCA and the LCC models to produce environmental and economic impacts. For detailed information about the methodology of each one, check the sections 4.2.2.3 and 4.3.2.3, respectively.

5.2.4. Multi-objective optimization

In this stage, the multi-objective optimization problem is formulated in synchrony with the predictive life cycle inventory and life cycle impact assessment phases. The main steps are shown in Figure 21.

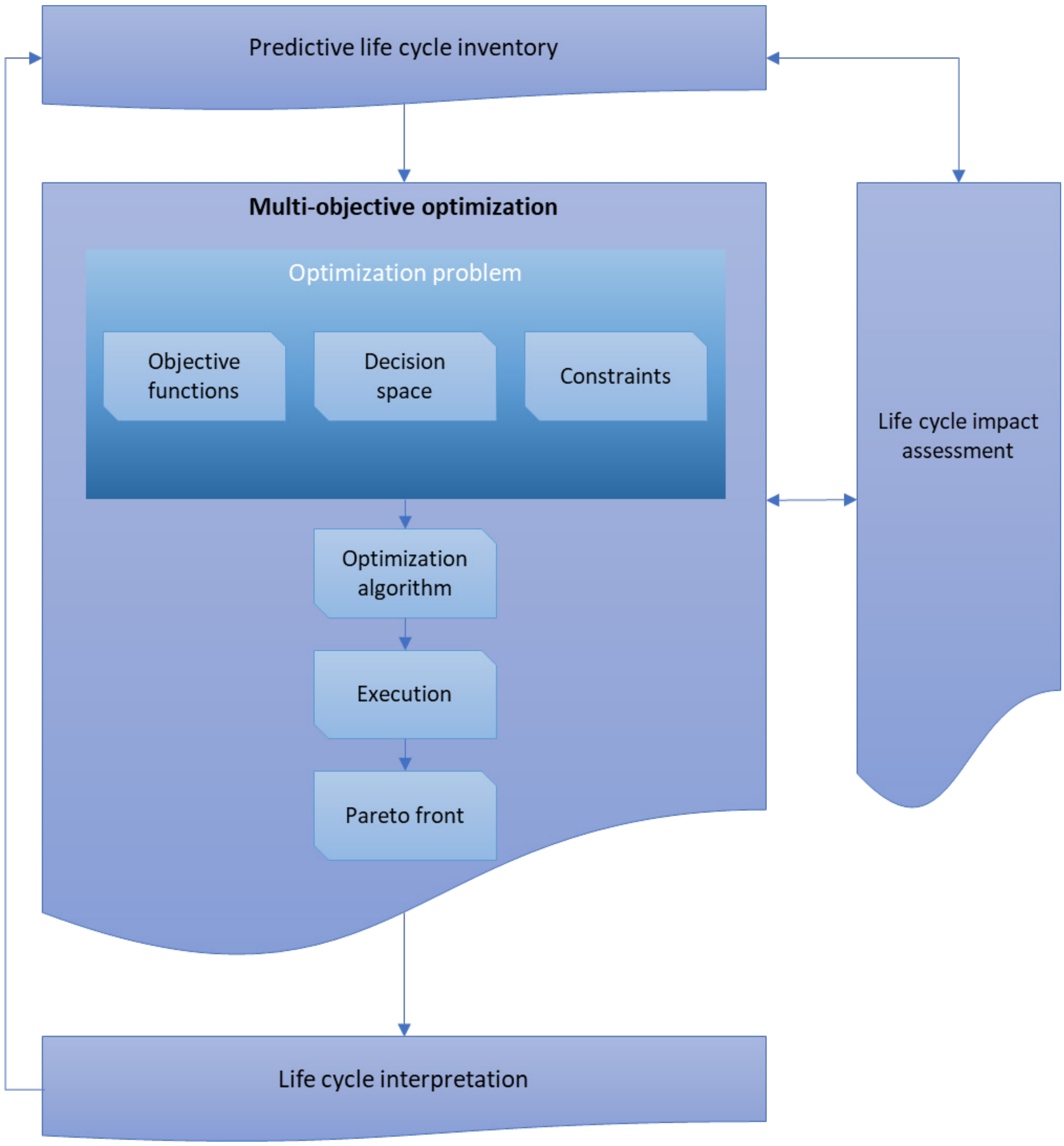

Figure 21. MOO problem in the eco-design framework for industrial processes

The objectives are defined from the predictive inventory (and, therefore, the simulation) and from the LCIA results. Furthermore, the decision space is defined by the design parameters and topological decisions in the simulation and life cycle models. Finally, technical constraints are encapsulated in the simulation model, while further constraints might be included in the problem depending on the results of previous framework phases or stakeholders' requirements to meet.

5.2.5. Life cycle interpretation

The life cycle interpretation phase comprises several elements: identification of the significant issues, an evaluation that considers completeness, sensitivity and consistency checks, and, finally, the conclusions, limitations and recommendations of the study. The relationship of the interpretation phase to other phases is shown in Figure 22.

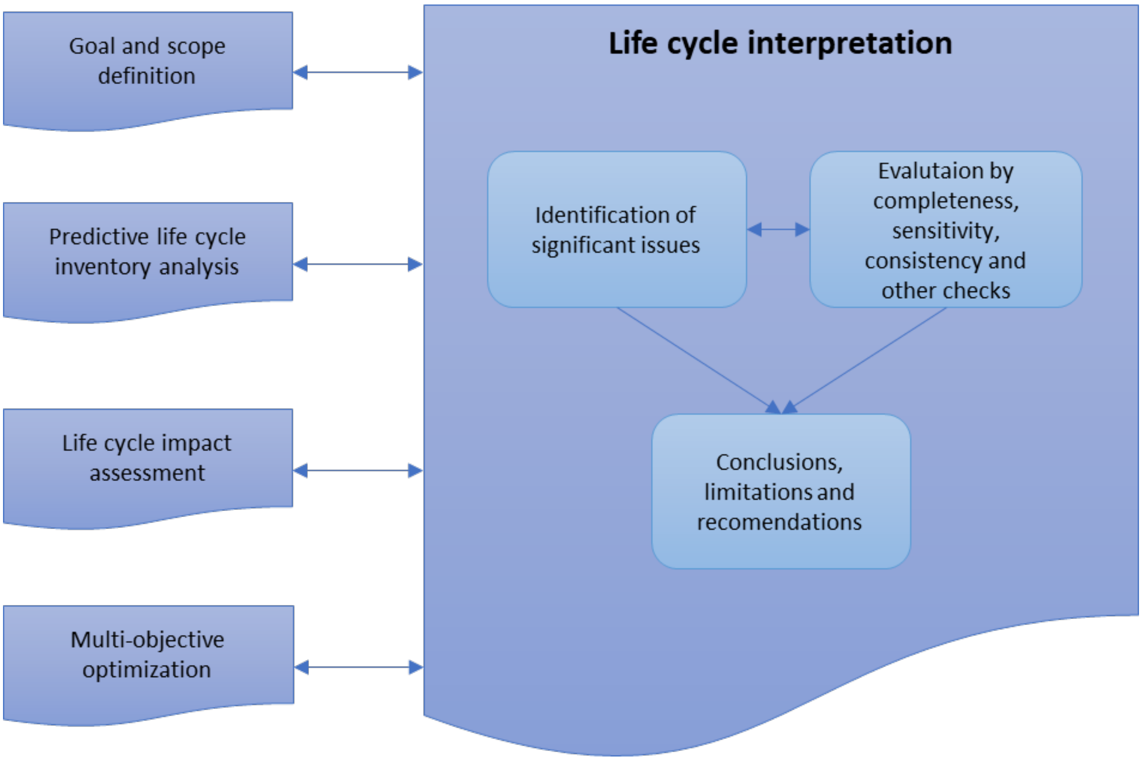

Figure 22. LCI phase in the eco-design framework for industrial processes

This phase together with the goal and scope stage of an eco-design project frame the study, while the other phases produce information on the optimal design for the industrial process under study.

5.2.5.1. Identification of significant issues

This element's mission is to organize the findings from the predictive inventory, LCIA and MOO phases in line with the goal and scope description to identify the key concerns. The main goal is to cover the effects of the techniques employed and assumptions made in the stages that came before it, including allocation guidelines, cut-off choices, impact category selection, category indicators, economic performance indicators, models selected in the process simulation, impact assessment method in the LCA, estimation model in the LCC, algorithm and problem definition in the MOO.

5.2.5.2. Evaluation

The goals of the evaluation element are establishing and enhancing confidence, as well as reliability, of the eco-design results; including the significant issues identified in the first element of the life cycle interpretation phase. The evaluation's findings should be presented so that any relevant stakeholder can easily grasp the conclusions of the study.

The use of the completeness and consistency checks shall be considered. However, the sensitivity check is crucial in the eco-design framework, not only to evaluate the reliability of the results and conclusions by identifying how uncertainties in the data affect them. But also, to refine the decision space which allows to improve the process simulation that will provide more reliable data to the LCA and LCC models.

5.2.5.3. Conclusions, limitations and recommendations

The objective of this part of the life cycle interpretation is to draw conclusions, identify limitations and make recommendations for the intended audience of the eco-design study on how to proceed when conducting a sustainability-based optimal design to the industrial process under study. This should be done iteratively with the other elements in the interpretation phase. Thanks to the inclusion of MOO to the eco-design framework this step is easier as many scenarios have been automatically evaluated by the optimization algorithm, while decision-makers only have to interpretate the results of the Pareto front and how the population have evolved during the optimization process. This way, decision-makers get better insights into the main hotspots of the system and how its sustainability performance behaves under different process conditions.

6. ECO-DESIGN TOOL FOR INDUSTRIAL PROCESSES: eco2des

6.1. Background

As concluded in Section 3, there is not only a need for a framework which integrates TEA, or process simulation plus LCC, with LCA and mathematical optimization; but also, and more conveniently, a tool working as a holistic and interoperable platform for encapsulating this framework easing the methodology application for any case study. There are several tools for performing process simulations, LCC, LCA and optimization separately, but, to our knowledge, there is not an integrated tool for the eco-design of industrial processes. That is why one of the main objectives of this thesis is to develop a pre-commercial version of that tool and with this premise, eco2des concept was born and is presented along this chapter.

6.2. Clarification

Due to the nature of the current thesis, a full disclosure of the developed code cannot be done. This thesis was developed into an industrial PhD program in which the industrial property belongs to the company involved in. The company has decided to keep the code under a commercial license; therefore, this section will provide a high-level description of the work done.

6.3. Introduction

In the future, process simulation will be increasingly more crucial as digitalization in the process engineering sector progresses. The complete data that simulation can provide about the current or potential states of the processes will permeate several higher-level applications and be used by a wider range of users as a result. Flowsheet simulations will thereby develop from a personal tool of the individual engineer for solving specific problems to an integral part of the technology stack (Sönke Bröcker et al. 2021) . As the relevant stakeholders, such as consumers and policymakers but also banks and investors, are also demanding more sustainable options, one key piece of this technology stack around process simulation will be environmental impacts computation, without leaving behind the economic performance of the industrial processes.

This advancement has a variety of implications for process simulation requirements. Connecting process simulation with other applications requires open interfaces, modularity, and effective data connectivity (Sönke Bröcker et al. 2021). Moreover, the use of process simulation in higher-level applications implicates additional demands such as higher accuracy, more robust convergence and faster computation times. With the development of eco2des, new solutions to these demands are foreseeable because it offers quick access to extensive information and very flexible choices for data-based modeling. eco2des is an object-oriented Python framework for sustainability-based optimization of industrial processes. The tool takes advantage of the full feature set of Python, such as its facilities for fast prototyping and the several available libraries for data processing, data analysis, scientific computing and data visualization. eco2des is a descriptive tool, which documents life cycle inventories and characterizes them through their environmental impact and associated costs. It is a predictive tool, since it uses as inputs physicochemical models for process simulation in the research phase; and adaptive, since it automates process design selections based on multi-objective optimization algorithms. As a result, the framework is able to take a process simulation, such an Aspen Plus file (Figure 23), linking it with LCA and LCC models and optimize its sustainable objectives changing operational variables, topology or supply chain decisions.

Figure 23. eco2des concept

6.4. eco2des architecture

eco2des has been designed having in mind developing a maintainable and scalable application, easy to adapt to new requirements and technologies that might appear in the future. Therefore, eco2des is formed of several modules (Figure 24), each one developed following an object-oriented paradigm.

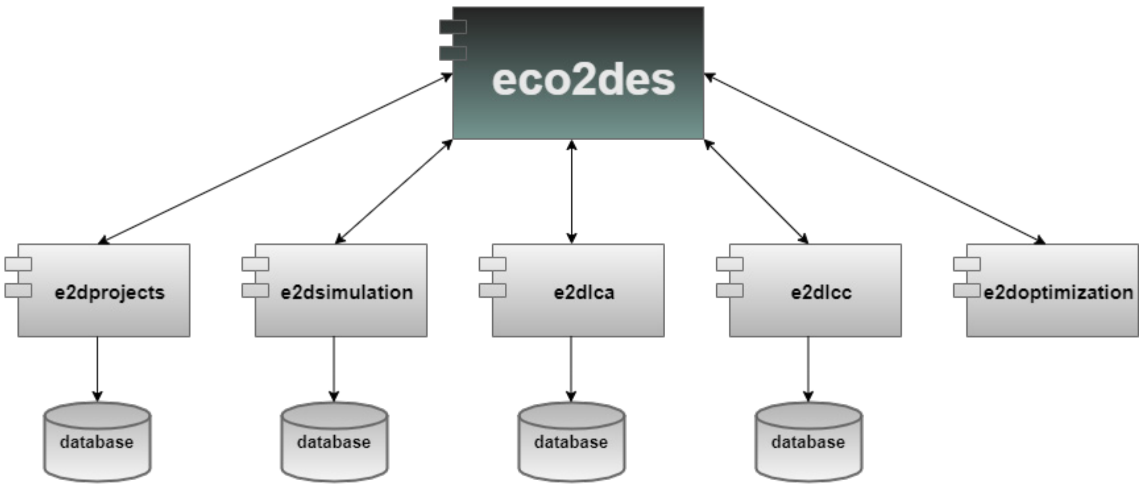

Figure 24. eco2des architecture scheme

This modularity has several advantages in spite of having a more complex system in terms of architecture design and communication between modules. However, there are huge benefits in terms of scalability. Not only each module can scale-up with new functionalities independently, but also new modules can be added to the framework drastically easier. As a result, eco2des is flexible and expandable, easing its deployment in private or public servers (cloud systems), as well as its integration with other frameworks or applications.

The core modules of eco2des are e2dprojects, e2dsimulation, e2dlca, e2dlcc and e2doptimization; all of them have an object-oriented design.

6.4.1. e2dprojects

The first module, e2dprojects, allows the user to create a new project, delete it, rename it and copy it, as well as to specify the current project in which the user is working on. A project is an entity which encapsulates a unique process simulation and its relations with its LCA model, its LCC model and its optimization problem. Project name, location, year, reference currency, system path (where results are stored), linked simulation, linked LCA, linked LCC and linked optimization problem are stored in a SQL database, in particular SQLite (SQLite Consortium 2022). Furthermore, projects are saved as directories in the filesystem where the actual simulation file, LCA database, and results, in form of byte objects, excel files or images are stored.

6.4.2. e2dsimulation

e2dsimulation module allows the user to interact with the simulation file linked to the project. There are methods for changing simulation inputs, running the simulation and reading results. To manage it, the module is linked to Windows programs through the Component Object Model (COM), using the Python library pywin32 (Hammond 2022). There is an abstract class, `ComConnection`, which other classes inherits from, such as `AspenPlusConnection` to interact with Aspen Plus. This design eases the implementation of other Windows programs in the future that are used in the computer aided process engineering. See Excurse 2 to have a better understanding of how to use COM interface to interact with Aspen Plus.

Excurse 2: The Variable Explorer in Aspen Plus. The Variable Explorer may be used to view and access variables and attributes associated with a specific Aspen Plus simulation file. Therefore, it is essential when carrying out automated operations with the COM interface. This is exposed by the Aspen Plus Automation library, apwn.dll or `Happ`, and the interface to interact with it is called `IHapp`.

The input and output data from an Aspen Plus simulation file are organized in a tree structure, which can be viewed and navigated using the Variable Explorer of the Aspen Plus User Interface (Figure 25).

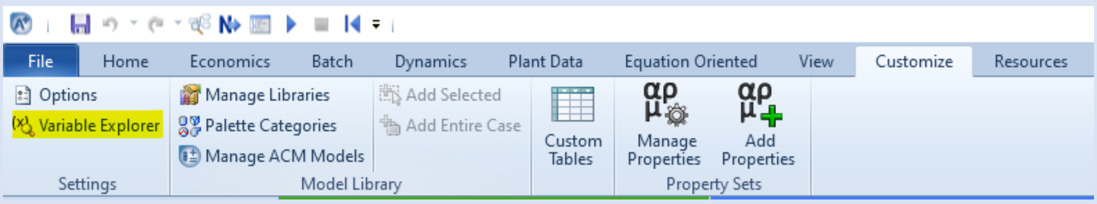

Figure 25. How to access the Variable Explorer in Aspen Plus v10.

The tree structure observed in the Variable Explorer reflects the information that is accessible via the COM interface as `IHNode` objects. Each node contains a value or data, or branches to another node (child).

The Objects Pane shows information of the nodes in the tree (Figure 26). The first node is called the root, which is returned by the Tree property of the `IHapp` interface. For instance, as shown in Figure 26, ANAME is a collection of node objects (`IHNodeCol`), hence it is a parent node, and the component CO is a single node object (`IHNode`), also called child and leaf as in this case it has no children. The dimension property of the different nodes defines how they are organized, for instance a dimension of 0 represents the last node on a branch, a leaf.

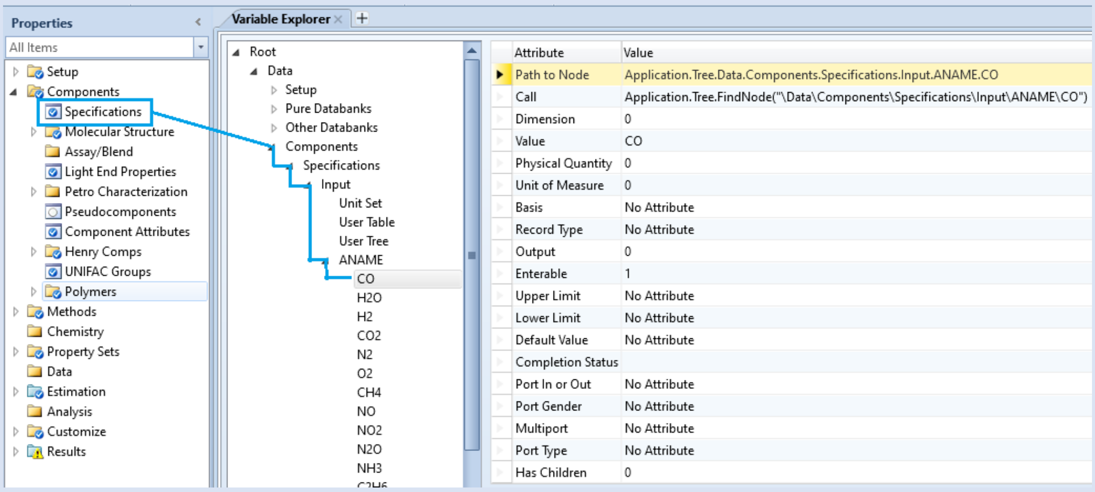

Figure 26. Navigation Pane, Objects Pane and Attributes Pane in Aspen Plus v10

Selecting an item in the Objects Pane displays it properties in the Attributes pane to the right. Attributes are enumerated as `HAP_` values (Figure 27).

Attribute	Value	
Path to Node	Application.Tree.Data.Components.Specifications.Input.ANAME.CO	
Call	Application.Tree.FindNode("\Data\Components\Specifications\Input\ANAME\CO")	
Dimension	0	IHNode.Dimension
Value	CO	IHNode.Value
Physical Quantity	0	HAP_UNITROW
Unit of Measure	0	HAP_UNITCOL
Basis	No Attribute	HAP_BASIS
Record Type	No Attribute	HAP_RECORDTYPE
Output	0	HAP_OUTVAR
Enterable	1	HAP_ENTERABLE
Upper Limit	No Attribute	HAP_UPPERLIMIT
Lower Limit	No Attribute	HAP_LOWERLIMIT
Default Value	No Attribute	HAP_VALUEDEFAULT
Completion Status		HAP_COMPSTATUS
Port In or Out	No Attribute	HAP_INOUT
Port Gender	No Attribute	HAP_PORTSEX
Multiport	No Attribute	HAP_MULTIPORT
Port Type	No Attribute	HAP_PORTTYPE
Has Children	0	HAP_HASCHILDREN

Figure 27. Attributes Pane in Aspen Plus v10

To access variables from the COM interface the Path to Node or Call attributes are used. The first is in dot notation, while the second uses the `FindNode` function call. Dot notation should be avoided as it does not always work as expected, especially when accessing user defined names.

Knowing how to navigate the Aspen Plus data tree using the Variable Explorer, it is easy to write a Python script that modifies simulation inputs, runs the simulation and retrieves results. For example, a simple Aspen Plus flowsheet representing a flash operation in which the FEED stream consists of 90 mol% of water and the rest ethanol at 21 °C and 50 psia, fed to the FLASH tank which is at 66 °C and 20 psia, producing two output streams, VAPOR and LIQUID. The Python script shown in Figure 28 uses that simulation file to modify the FLASH temperature, run a simulation, store the ethanol mole fraction that each output stream has and, finally, plot the results for data visualization.

```python
import numpy as np
import matplotlib.pyplot as plt
import win32com.client as win32

SIMULATION_FPATH = "data/flash.bkp"
RESULT_FPATH = "data/results.png"

# Initialize the COM interface and reading the simulation

aspen = win32.Dispatch("Apwn.Document")
aspen.initFromArchive2(SIMULATION_FPATH)

# Create a vector of temperatures from 66 C to 94 C

temperatures = np.linspace(66, 94, 2)

# Create a list to store mole fraction results

liquid_ethanol, vapor_ethanol = [], []

# Run the simulation and retrieve results for the different temperatures

for temperature in temperatures:
    aspen.Tree.FindNode("\Data\Blocks\FLASH\Input\TEMP").Value = temperature
    aspen.Engine.Run2()
    liquid_ethanol.append(
        aspen.Tree.FindNode("\Data\Streams\LIQUID\Output\MOLEFRAC\MIXED\ETHANOL").Value
    )
    vapor_ethanol.append(
        aspen.Tree.FindNode("\Data\Streams\VAPOR\Output\MOLEFRAC\MIXED\ETHANOL").Value
    )

# Create a plot of the results and saving it

plt.plot(temperatures, liquid_ethanol, vapor_ethanol)
plt.legend(["liquid", "vapor"])
plt.xlabel("Flash Temperature (Celsius)")
plt.ylabel("Ethanol mole fraction")
plt.savefig(RESULT_FPATH)

# Close the aspen connection

aspen.close()
```

Figure 28. Illustrative Python script to automate Aspen Plus using the COM interface.

When a simulation file is loaded into an eco2des project, e2dsimulation module traverses the Aspen Plus data tree (aka Variable Explorer tree) and stores the different simulation entities in the eco2des simulation object. Right now, eco2des supports the following Aspen Plus entities:

- Components.

- Streams, in particular material streams.
- Blocks, having support for RPlug, Heater, HeatX, Mixer, FSplit, Flash2, Decanter, Sep, RGibbs, Pump and Compr.
- Utilities.
- DesignSpecs.
- Calculators.

All the Aspen Plus entities inherit from the same class, `SimulationEntity` (Figure 29), that defines the shared attributes: the entity name, the path to the node in the Aspen Plus data tree and two objects, inputs and outputs. The inputs object is where the modifications are done to be reflected in the simulation file, while the outputs object is where data is read after the simulation is solved.

```python
@dataclass
class SimulationEntity:
    name: str
    path: str
    inputs: SimulationEntityInput
    outputs: SimulationEntityOutput

```

Figure 29. SimulationEntity class in Python pseudo code.

Components are represented by the `Component` class which is a wrapper for the different components defined in the simulation. This way eco2des knows the user defined components and therefore is able to access, for example, their composition in the different simulation streams.

For material streams, there is a `MaterialStream` wrapper class which inherit from the generic `Stream` class (which inherits from `SimulationEntity`). This eases the future implementation of new classes, such as `HeatStream` and `WorkStream`, to handle all the Aspen Plus stream types. `MaterialStream` class has methods to modify the total flow, the stream composition, the temperature, the pressure and the vapor fraction of a material stream. Furthermore, it retrieves for all the material streams in the simulation data about their mass flow, volume flow and mole flow by component, as well as their temperature, pressure and vapor fraction.

All defined blocks in eco2des inherit from the generic `Block` class. Furthermore, there are classes for interacting with each one of them such as the `FSplitBlock` class that has methods for changing the split fraction in this particular simulation block or reading the output pressure.

Class `Utility` wraps the homonymous simulation block and allows the user to retrieve utility usage values for the different simulation blocks.

Finally, there are two wrapper classes for two flowsheeting option entities, design specs and calculators. The first is wrapped in the `DesignSpec` class which has setter methods to change the specification in terms of flowsheet variables, and the target value for the spec expression. The last is modelled in the `Calculator` class, it only works with Fortran calculators allowing the user to change lines of code in the Fortran calculator giving the integer that represents the line number and the string value to replace it.

All these entities are stored in the simulation object of eco2des, it is an instance of the class `Simulation` which has several mapping objects that allows the user to retrieve the different simulation entities, using as keys the name of the entities and as values the instances of the corresponding object that wraps that simulation entity. These mapping objects are populated when the simulation file is loaded. Furthermore, the different entity objects are mapped to documents that are stored in different collections in a MongoDB database (MongoDB 2022), using the PyMongo library (MongoDB [2009] 2022). This way, the state of the simulation in eco2des is preserved without messing with the actual simulation file which always preserves its original state as when it is loaded into the tool.

6.4.3. e2dlca

The module responsible of assessing the environmental impacts of an industrial process is e2dlca. It inherits the most of its capabilities from Brightway2 (Mutel 2017), an open-source framework for life cycle assessment calculations in Python. Hence, e2dlca module is able to solve a matrix based LCA (Heijungs and Suh 2002), using more than 700 life cycle impact assessment methods that work with ecoinvent 2 and 3 databases (Frischknecht et al. 2005). Furthermore, the user may import its own inventory databases, having integrated support for the most standardized in the state-of-the-art studies such as ecoinvent 3 (Wernet et al. 2016), if the user has a license. For further information about the matrix based LCA calculation, see Excurse 3.

Excurse 3: Matrix based LCA calculation. To solve an LCA model using a matrix-based approach the product system must be modeled in terms of linear algebra, then the linear system may be reformulated using matrices.

The main matrices in a LCA model are:

- $\boldsymbol{A} \in Mat_R(m \, x \, n)$, the technosphere matrix or technology matrix, which describes the links among activities in the technosphere. These exchanges, a_{ij} represent the direct requirements of product i to produce 1 unit of product j.
- $\boldsymbol{B} \in Mat_R(l \, x \, n)$, the biosphere matrix or satellite matrix or intervention matrix, describing the exchanges between the activities and the environment (elementary flows). The elements b_{ij} represent the direct emissions (+) or resources (-) of elementary flows needed to produce 1 unit of product j.

- $\boldsymbol{C} \in Mat_R(k\ x\ l)$, the characterization matrix, whose elements c_{ij} represent the characterization factor of the elementary flow j for each k impact category.
- $\boldsymbol{f} \in Mat_R(m\ x\ 1)$, the final demand vector, which represents the reference product of the system.

The only condition to solve a matrix based LCA is that the equation $\boldsymbol{As} = \boldsymbol{f}$ must be solvable, being the vector $\boldsymbol{s} \in Mat_R(m\ x\ 1)$ the scaling vector. Then, $\boldsymbol{g} = \boldsymbol{Bs}$ is the inventory result for the final demand $\boldsymbol{f}$ of the product system, with $\boldsymbol{g} \in Mat_R(l\ x\ 1)$. Finally, the inventory may be characterized as follows $\boldsymbol{h} = \boldsymbol{gC}$, where $\boldsymbol{h} \in Mat_R(k\ x\ 1)$ are the LCIA results for each impact category.

Furthermore, to perform additional studies such as upstream analysis, an additional condition is needed. Hence, matrix $\boldsymbol{A}$ must be invertible. As $\boldsymbol{A}^{-1}$ represents the total requirements (direct and upstream) of product i to produce 1 unit of product j. Therefore, the intensity matrix, $\boldsymbol{M} \in Mat_R(l\ x\ n)$, may be calculated as $\boldsymbol{M} = \boldsymbol{BA}^{-1}$ which includes the total LCI results for a final demand of 1 unit of the j^{th} product. The intensity matrix is needed to compute upstream contributions of the product system.

Brightway2 offers capabilities to store and search all relevant data sources in an LCA study, such as environmental databases and LCIA methods. Besides, it has a matrix builder that translates the environmental data into the technosphere and biosphere matrices, the first one has the information of all the input/output direct relationships between the technosphere activities and the last represents the direct emissions and natural resources needed by each one of the technosphere activities. Furthermore, Brightway2 can solve the linear system to perform LCA calculations and, finally, has several capabilities to analyze the results. All these functionalities are encapsulated in the `lca` object exposed by eco2des.

However, every time that Brightway2 performs a calculation it has to read from the environmental databases and build the matrices. In a case in which ecoinvent 3 is used as background database, it means to perform more than 18,000 I/O operations to retrieve each ecoinvent activity plus for each one of them their exchanges need to be joined as well to build the technosphere and biosphere matrices. It converts the LCA calculation into an I/O bound operation whose speed is limited by the I/O subsystem. This is a particular concern for eco2des, as solving a multi-objective optimization problem means to evaluate thousands of different scenarios and repeat the matrix building step in each evaluation would have a huge negative impact in the tool performance.

Therefore, to avoid this problem e2dlca module is able to cache these matrices in memory. Besides, it saves index references to the activity/product pair in a mapping object whose keys are the activity/product reference, and the values are the integer index in the square technosphere matrix representing the row or the column. For the biosphere matrix, an additional mapping object is needed that has the elementary flow reference as keys and the appropriate index pointing to the matrix element as value. Therefore, new simulation results might be available in each evaluation and instead of modifying the linked technosphere or biosphere exchanges in the database and rebuilding the matrices, what is done is actually overwrite the matrix elements with new values in the cache and directly solve the new linear system.

As an example, given the following technosphere matrix, where act means activity:

$$\boldsymbol{A} = \begin{array}{c} \\ act\ 1 \\ act\ 2 \\ act\ 3 \end{array} \begin{array}{c} \begin{array}{ccc} act\ 1 & act\ 2 & act\ 3 \end{array} \\ \begin{bmatrix} 1 & -0.1 & -0.6 \\ 0.1 & 1 & -0.2 \\ 0 & 0 & 1 \end{bmatrix} \end{array}$$

The mapping object would look like the Python dictionary in Figure 30.

```
TECHNOSPHERE_MAPPING = {
        "activity 1": 0,
        "activity 2": 1,
        "activity 3": 2,
}
```

Figure 30. Indices for the technosphere matrix example.

Hence, if our product system under analysis is the activity 3 and we might want to modify its exchange with the activity 2 value from -0.2 to -0.3, we can do it directly in the matrix following this strategy which drastically improves computation speed.

Finally, to support the life cycle interpretation phase, e2dlca has several postprocessing functionalities to analyze the results using data visualization libraries such as matplotlib (Hunter 2007) and plotly (Inc 2015). The main interpretation functionalities are visualizing top elementary flow contributors (Figure 31), visualizing top process contributors (Figure 32) and visualizing an interactive Sankey diagram for analyzing upstream contributions (Figure 33).

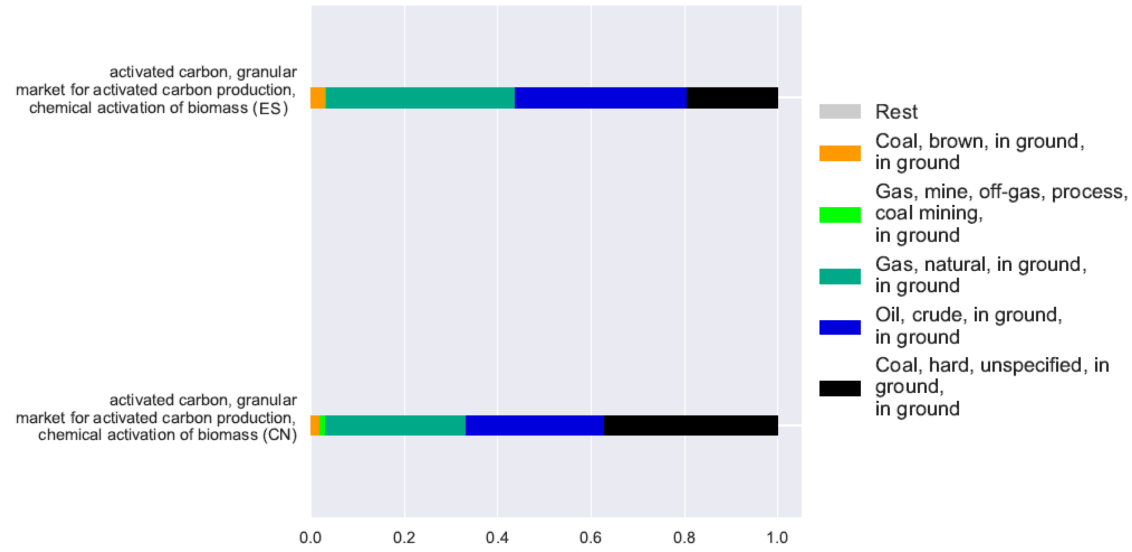

Figure 31. Top elementary flow contributors to ReCiPe Midpoint (H) fossil depletion impact category of two processes using eco2des.

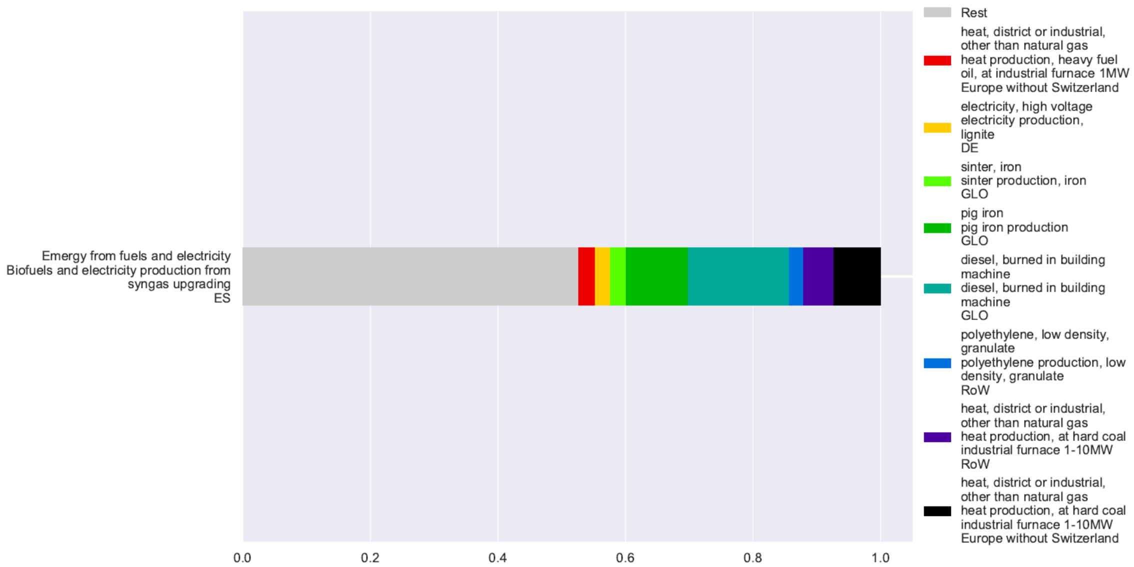

Figure 32. Top process contributors to ReCiPe Midpoint (H) climate change (GWP500) impact category of one process using eco2des.

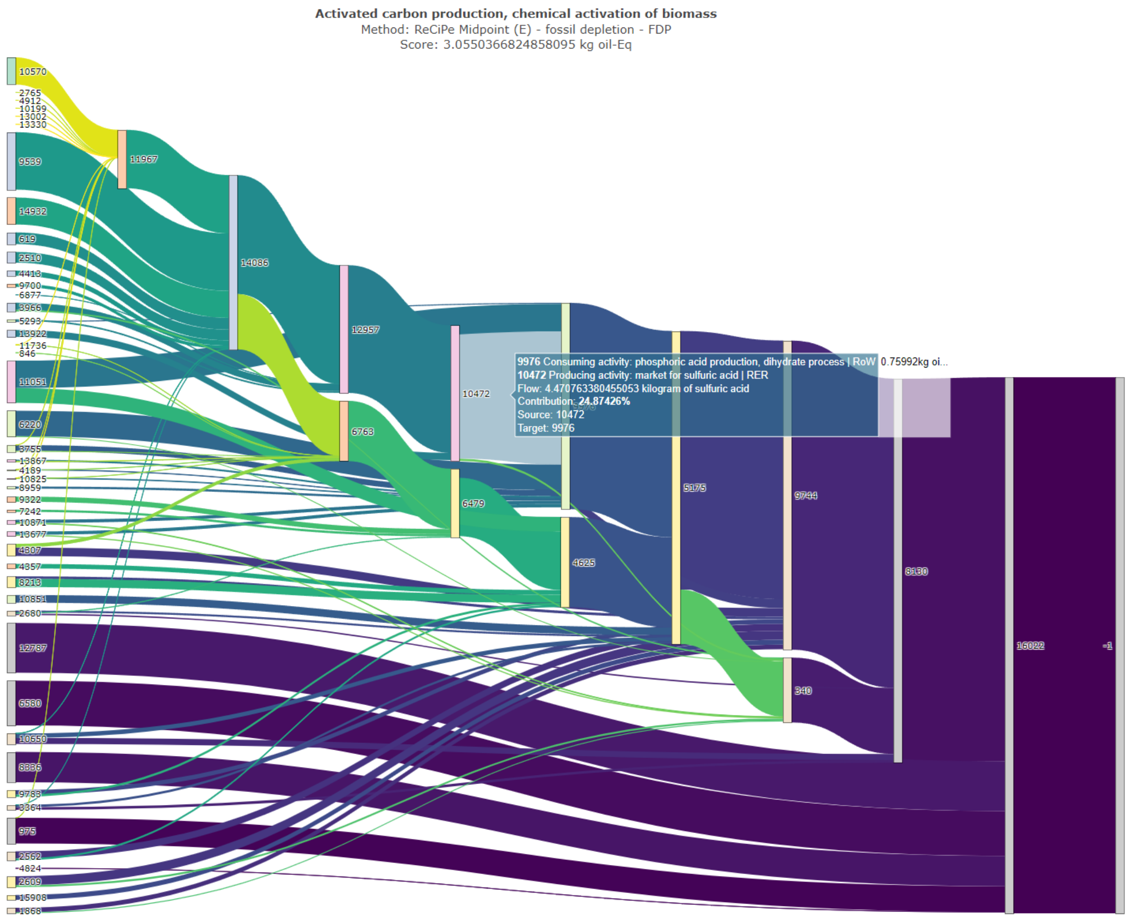

Figure 33. Interactive Sankey diagram for upstream contribution analysis in eco2des.

6.4.4. e2dlcc

The assessment of the process life cycle costing is carried out by the e2dlcc module. It solves a conventional LCC using a cradle-to-gate system boundary as explained in Section 4.3.2. e2dlcc creates an `lcc` object which is exposed by the eco2des application interface. This object has methods for computing the CAPEX, the OPEX and a cash-flow model for an industrial process.

First, a class `Capex` is in charge of estimating the capital investment. It has several factory methods to create the different plant equipment objects and store them in a collection. To estimate the purchased equipment costs, e2dlcc offers several methods. On the one hand, it includes cost curves in the form of:

$$C_e = a + bS^n \quad (5)$$

Where:

- C_e is the purchased equipment cost on a U.S. Gulf Coast basis, January 2010
- a, b are the cost constants
- S is the size parameter
- n is the exponent for that type of equipment

These correlations were extracted from (Towler and Sinnott 2013a) and the ones included in eco2des are shown in Table 1.

Table 1. Purchased equipment cost correlations in eco2des (Based on Towler and Sinnott 2013)

Equipment	***Units for S***	S_{lower}	S_{upper}	***a***	***b***	***n***
Agitators and mixers						
Propeller	Driver power, kW	5.0	75	17,000	1.13	1.05
Spiral ribbon mixer	Driver power, kW	5.0	35	30,800	125	2.0
Static mixer	liters/s	1.0	50	570	1,170	0.4
Boilers						
Packaged, 15 to 40 bar	kg/h steam	5,000	200,000	124,000	10.0	1.0
Field erected, 10 to 70 bar	kg/h steam	20,000	800,000	130,000	53	0.9
Centrifuges						
High speed disk	diameter, m	0.26	0.49	57,000	480,000	0.7
Atmospheric suspended basket	power, kW	2.0	20	65,000	750	1.5
Compressors						
Blower	m^3/h	200	5,000	4,450	57	0.8
Centrifugal	Driver power, kW	75	30,000	580,000	20,000	0.6
Reciprocating	Driver power, kW	93	16,8000	260,000	2,700	0.75
Conveyors						
Belt, 0.5 m wide	length, m	10	500	41,000	730	1.0
Belt, 1.0 m wide	length, m	10	500	46,000	1,320	1.0
Bucket elevator, 0.5 m bucket	height, m	10	30	17,000	2,600	1.0
Crushers						
Reversible hammer mill	t/h	30	400	68,400	730	1.0
Pulverizers	kg/h	200	4,000	16,000	670	0.5
Jaw crusher	t/h	100	600	−8,000	62,000	0.5
Gyratory crusher	t/h	200	3,000	5,000	5,100	0.7
Ball mill	t/h	0.7	60	−23,000	242,000	0.4

Crystallizers						
Scraped surface crystallizer	length, m	7	280	10,000	13,200	0.8
Dryers						
Direct contact Rotary	m^2	11	180	15,000	10,500	0.9
Atmospheric tray batch	area, m^2	3.0	20	10,000	7,900	0.5
Spray dryer	Evaporation rate kg/h	400	4,000	410,000	2,200	0.7
Evaporators						
Vertical tube	area, m^2	11	640	330	36,000	0.55
Agitated falling film	area, m^2	0.5	12	88,000	65,500	0.75
Exchangers						
U-tube shell and tube	area, m^2	10	1,000	28,000	54	1.2
Floating head shell and tube	area, m^2	10	1,000	32,000	70	1.2
Double pipe	area, m^2	1.0	80	1,900	2,500	1.0
Thermosiphon reboiler	area, m^2	10	500	30,400	122	1.1
U-tube Kettle reboiler	area, m^2	10	500	29,000	400	0.9
Plate and frame	area, m^2	1.0	500	1,600	210	0.95
Filters						
Plate and frame	capacity, m^3	0.4	1.4	128,000	89,000	0.5
Vacuum drum	area, m^2	10	180	–73,000	93,000	0.3
Furnaces						
Cylindrical	duty, MW	0.2	60	80,000	109,000	0.8
Box	duty, MW	30	120	43,000	111,000	0.8
Packings						
304 ss Raschig rings	m^3			0	8,000	1.0
Ceramic intalox saddles	m^3			0	2,000	1.0
304 ss Pall rings	m^3			0	8,500	1.0
PVC structured packing	m^3			0	5,500	1.0
304 ss structured packing	m^3			0	7,600	1.0
Pressure vessels						
Vertical, cs	Shell mass, kg	160	250,000	11,600	34	0.85
Horizontal, cs	Shell mass, kg	160	50,000	10,200	31	0.85
Vertical, 304 ss	Shell mass, kg	120	250,000	17,400	79	0.85
Horizontal, 304 ss	Shell mass, kg	120	50,000	12,800	73	0.85
Pumps and drivers						
Single stage centrifugal	flow, liters/s	0.2	126	8,000	240	0.9
Explosion proof motor	power, kW	1.0	2,500	–1,100	2,100	0.6
Condensing steam turbine	power, kW	100	20,000	–14,000	1,900	0.75
Reactors						
Jacketed, agitated	volume, m^3	0.5	100	61,500	32,500	0.8

Jacketed, agitated, glass lined	volume, m^3	0.5	25	12,800	88,200	0.4
Tanks						
Floating roof	capacity, m^3	100	10,000	113,000	3,250	0.65
Cone roof	capacity, m^3	10	4,000	5,800	1,600	0.7
Trays						
Sieve trays	diameter, m	0.5	5.0	130	440	1.8
Valve trays	diameter, m	0.5	5.0	210	400	1.9
Bubble cap trays	diameter, m	0.5	5.0	340	640	1.9
Distillation columns						
From pressure vessels, packaging and trays						
Utilities						
Cooling tower and pumps	flow, liters/s	100	10,000	170,000	1,500	0.9
Packaged mechanical refrigerator evaporator	duty, kW	50	1,500	24,000	3,500	0.9
Water ion exchange plant	Flow m^3/h	1	50	14,000	6,200	0.75

In addition to these correlations, e2dlcc can also estimate the equipment cost using a cost curve method. This is useful as it is common to find references for an equipment cost of a specific capacity. Then, if the scaling factor between capacities is also known, the cost of the equipment may be estimated as follows:

$$Cost = Cost_{reference}\left({Capacity}/{Capacity_{reference}}\right)^{scale\ factor} \quad (6)$$

To conclude equipment cost estimation, the user may also directly provide a cost for a specific equipment. Furthermore, when a cost is estimated using one of the correlations in Table 1, the cost is related to January 2010 in US dollars. Therefore, it might need to be updated using equation 4. To do so, e2dlcc uses, as price index, the average annual Chemical Engineering Plant Cost Index, CEPCI (Jenkins 2022) for the equipment cost year and the eco2des project year. Also, the equipment cost might need to be exchanged into the reference currency defined in the project level. Both, CEPCI and exchange rates data for euros and US dollars, are stored in a SQLite database (SQLite Consortium 2022).

Once all the purchased equipment costs are estimated, e2dlcc estimates the installed costs using a detailed factorial method (Towler and Sinnott 2013a). However, it is not applied for the equipment cost estimations that already include erection costs. Using this method, the following incurred costs during the construction of a plant are estimated:

- Equipment erection, including foundations and minor structural work.
- Piping, including insulation and painting.
- Electrical, power and lighting.
- Instruments and automatic process control (APC) systems.
- Process buildings and structures.
- Ancillary buildings, offices, laboratory buildings, workshops.
- Storage for raw materials and finished product.
- Utilities, provision of plant for steam, water, air, firefighting services.
- Site preparation.

Then, the following equations are used to compute the ISBL costs:

$$C = \sum_{i=1}^{i=M} C_{e,i,CS}\left[\left(1+f_p\right)f_m + \left(f_{er}+f_{el}+f_i+f_c+f_s+f_l\right)\right] \quad (7)$$

$$C = \sum_{i=1}^{i=M} C_{e,i,A}\left[\left(1+f_p\right) + \frac{\left(f_{er}+f_{el}+f_i+f_c+f_s+f_l\right)}{f_m}\right] \quad (8)$$

$$ISBL = \sum C \quad (9)$$

Where:

- $C_{e,i,CS}$, purchased equipment cost of equipment i in carbon steel
- $C_{e,i,A}$, purchased equipment cost of equipment i in another material
- M, total number of equipment's pieces
- f_p, installation factor for piping
- f_{er}, installation factor for equipment erection
- f_{el}, installation factor for electrical work
- f_i, installation factor for instrumentation and process control

- f_c, installation factor for civil engineering work
- f_s, installation factors for structures and buildings
- f_l, installation factor for lagging, insulation, or paint
- f_m, material factor

Equation 7 is used when the purchased equipment cost has been estimated on a carbon steel basis. However, when this cost is estimated in a different material basis, equation 8 is used instead. Installation factors and material cost factors are shown in Table 2 and Table 3.

Table 2. Factors for estimating installation costs in eco2des (Based on Towler and Sinnott 2013)

Item	Process Type		
	Fluids	Fluids and solids	Solids
f_{er}	0.3	0.5	0.6
f_p	0.8	0.6	0.2
f_i	0.3	0.3	0.2
f_{el}	0.2	0.2	0.15
f_c	0.3	0.3	0.2
f_s	0.2	0.2	0.1
f_l	0.1	0.1	0.05
f_{OSBL}	0.3	0.4	0.4
$f_{D\&E}$	0.3	0.25	0.2
f_X	0.1	0.1	0.1

Having estimated the ISBL cost, factors for estimating the OSBL, Design and Engineering (D&E) and contingency (X) costs are used as follows (see Table 2):

$$OSBL = ISBL(1 + f_{OSBL}) \qquad (10)$$

$$D\&E = ISBL(1 + f_{D\&E}) \qquad (11)$$

$$X = ISBL(1 + f_X) \qquad (12)$$

Then the CAPEX of the project is:

$$CAPEX = ISBL + OSBL + D\&E + X \qquad (13)$$

Table 3. Materials cost factors relative to carbon steel in eco2des (Based on Towler and Sinnott 2013)

Material	f_m
Carbon steel	1.0
Aluminum and bronze	1.07
Cast steel	1.1
304 stainless steel	1.3
316 stainless steel	1.3
321 stainless steel	1.5
Hastelloy C	1.55
Monel	1.65
Nickel and Inconel	1.7

Finally, to get the total investment required, fixed and working capital cost to erect the plant might be added by the user specifying a percentage of the CAPEX to compute its estimation. Typically, this value is in a range of 10 % to 20 % (Towler and Sinnott 2013a).

The next step performed by e2dlcc is the estimation of the project's OPEX. To that purpose, it applies a percentage method based on CAPEX estimations as shown in Table 4. The user can modify these percentages and the values are stored in the project level. All this logic is encapsulated into the class `Opex`.

Inputs from the user are needed to model operating labor, capital charges, raw materials and utilities costs, and link its calculation to the outputs from the process simulation inserted in the project.

Finally, e2dlcc module allows the user to build a financial LCC model which computes net present value, internal rate of return, payback or levelized cost of production among other economic performance indicators. To do so, a method is exposed by the module and the user needs to provide CAPEX and OPEX objects, as well as, the plant lifetime, the discount rate and the plant erection time.

Table 4. OPEX calculations in eco2des

Fixed costs	Maintenance	$5\% \cdot ISBL$
	Operating labour	$defined\ by\ user$
	Supervision	$25\% \cdot Operating\ labour$
	Plant overheads	$65\% \cdot (Operating\ labour + Supervision)$
	Capital charges	$loan\ conditions\ and\ depreciation\ defined\ by\ user$
	Environmental costs	$1\% \cdot (ISBL + OSBL)$
	Insurance	$1\% \cdot ISBL$
	License fees and royalties	$2.5\% \cdot Sales$
Variable costs	Raw materials	$linked\ to\ process\ simulation\ outputs$
	Utilities	$linked\ to\ process\ simulation\ outputs$
	Operating materials	$10\% * Maintenance$

As e2dlca module, e2dlcc also provides functionalities to support the life cycle interpretation phase for economic data. Hence, the tool has methods to export results to excel and to visualize them. Some visualization examples are shown in Figures 34, 35, 36 and 37.

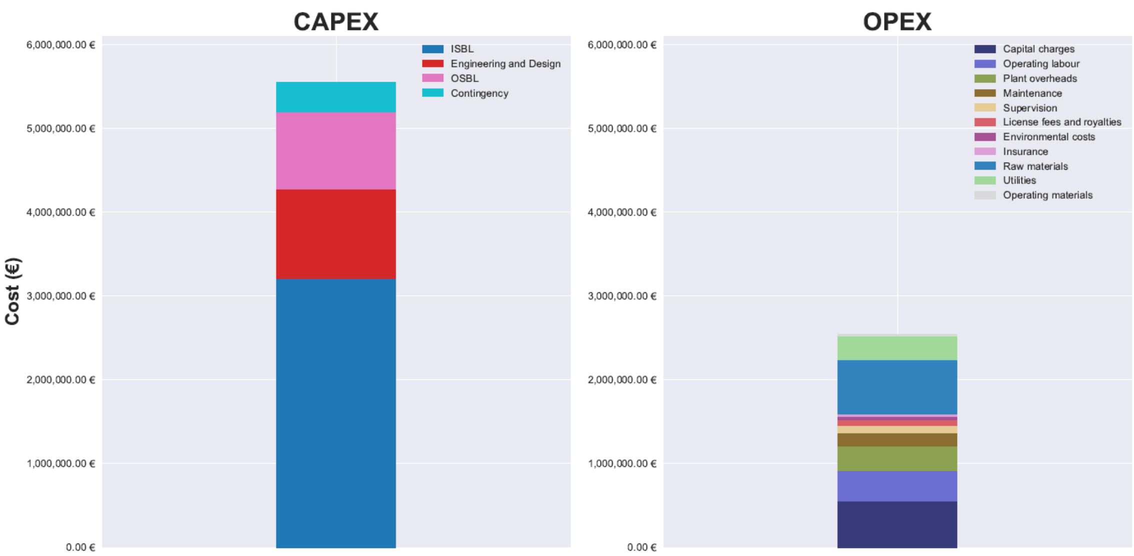

Figure 34. CAPEX vs annual OPEX costs from eco2des.

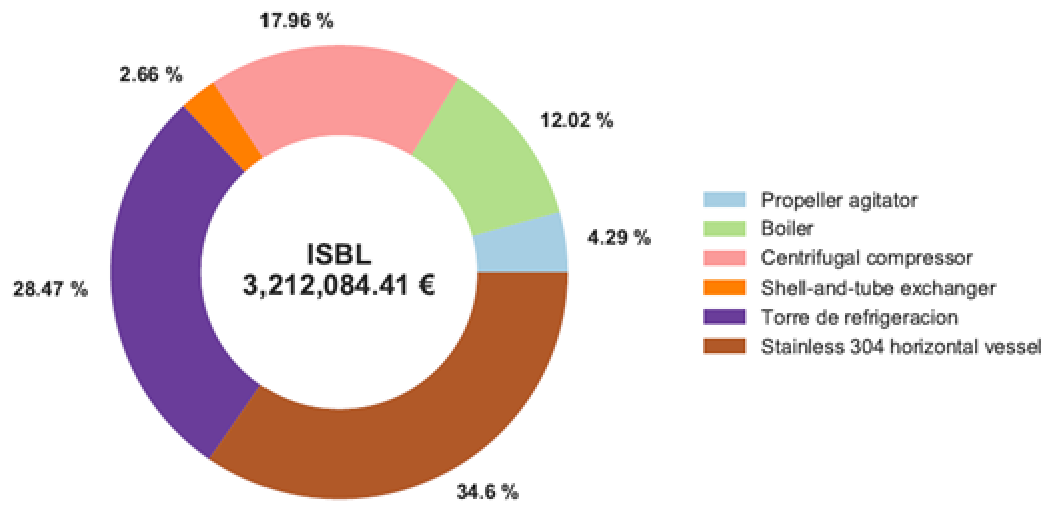

Figure 35. ISBL costs visualization from eco2des.

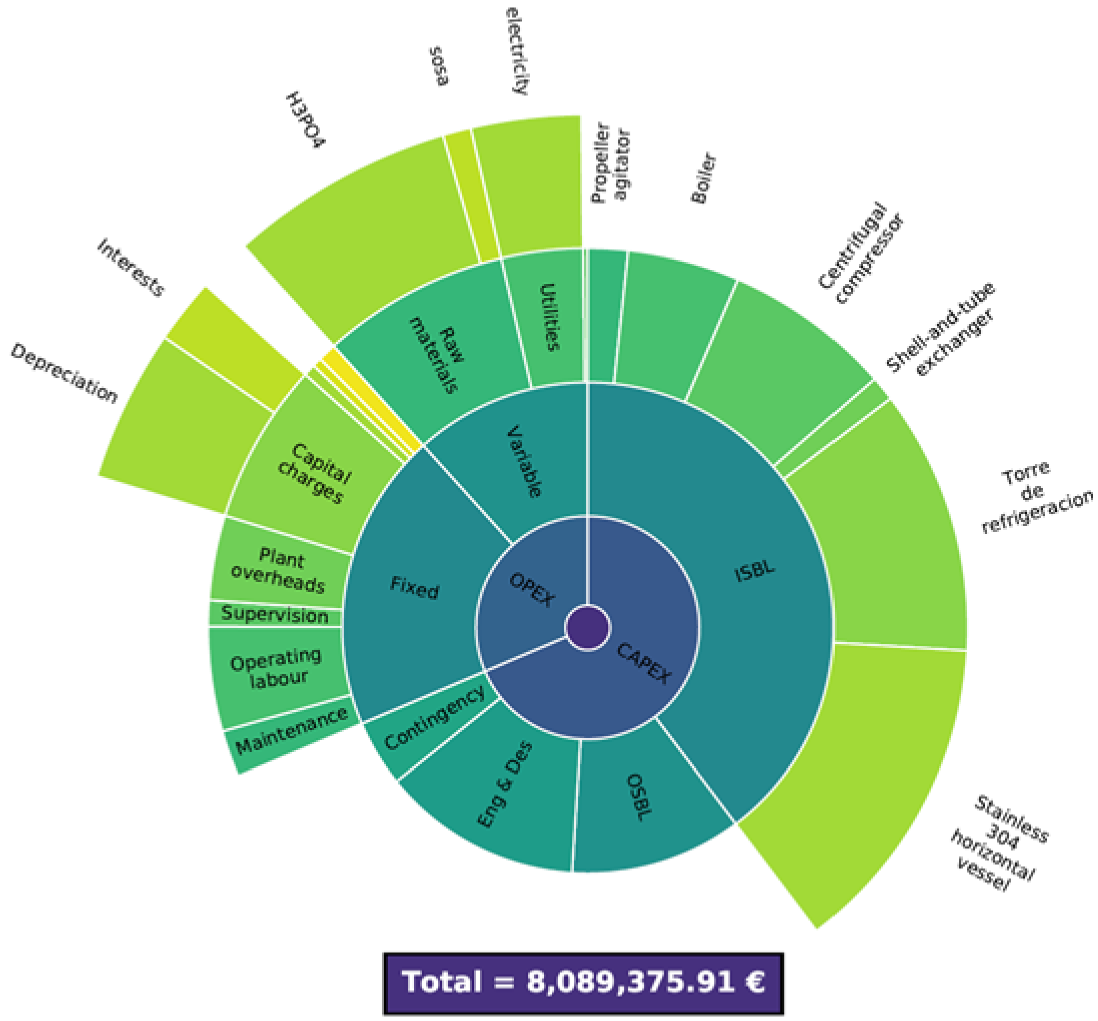

Figure 36. Sunburst visualization of the main project costs from eco2des.

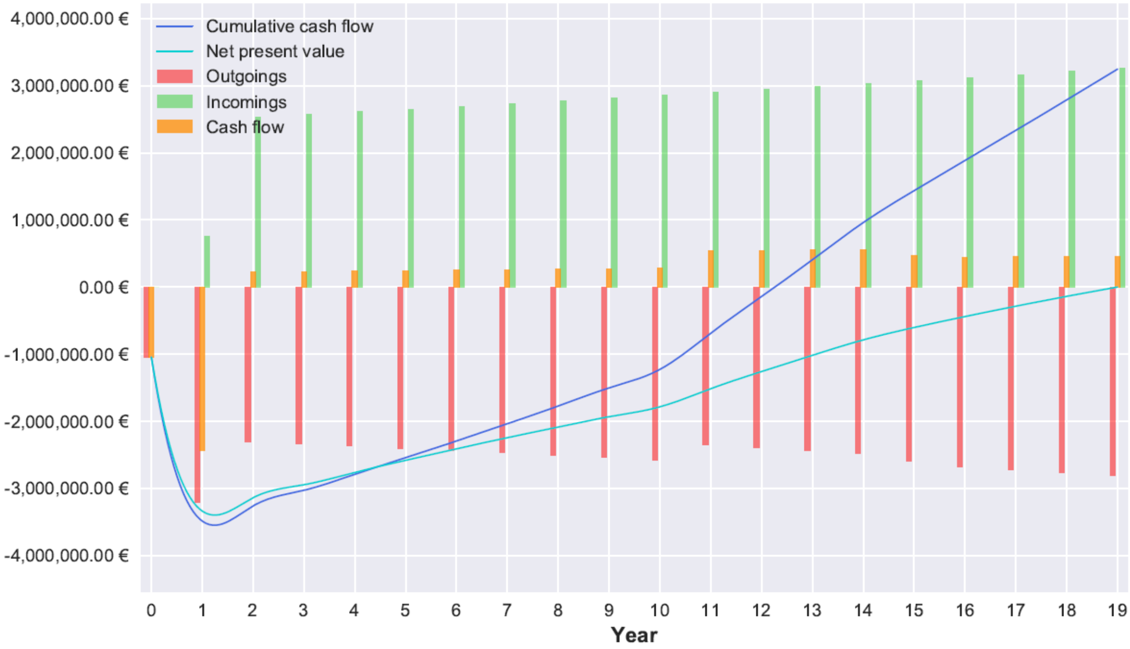

Figure 37. Financial model results visualization from eco2des.

6.4.5. e2doptimization

The last module in the framework is e2doptimization, it exposes an `optimization` object that allows the user to define the optimization problem to solve, selecting the decision variables from process simulation, LCA model and/or LCC model; their boundaries, the problem constrains and the objectives from the three abovementioned entities. This module has several algorithms for heuristic global optimization (Table 5), with single or multiple objectives. For a brief explanation of those, check the Excurse 4. These algorithms are taken from pygmo (Biscani and Izzo 2020).

Excurse 4: Optimization algorithms in eco2des.

- **Extended Ant Colony Optimization (GACO)**

GACO is an innovative optimization algorithm to address non-convex mixed integer nonlinear programming (MINLP) problems. The GACO algorithm is an extension of traditional Ant Colony Optimization (ACO) and combines the principles of artificial ants with penalty functions to manage continuous and integer variables. In GACO, artificial ants construct solutions by traversing the decision space, guided by pheromone trails and heuristic information.

The algorithm employs a dynamic penalty function to enforce the feasibility of solutions and manage the trade-off between exploration and exploitation. Additionally, it introduces a local search strategy to improve the quality of the solutions found by the ants.

- **Differential Evolution (DE)**

DE is a powerful optimization algorithm that efficiently solves global optimization problems. DE is a population-based, stochastic search method that excels in handling continuous, non-linear, and non-convex objective functions with a high degree of robustness and adaptability. The DE algorithm operates through the generation of trial solutions using mutation, crossover, and selection operators. Mutation is achieved by adding a scaled difference vector between two randomly chosen population members to a third member, resulting in a new candidate solution. The crossover operation combines elements from the mutated vector and the original target vector to create a trial vector, which then competes against the target vector based on their fitness values in the selection process.

- **Self-adaptative differential Evolution (iDE)**

iDE is an advanced optimization algorithm to address real-world numerical optimization problems. iDE enhances the traditional Differential Evolution (DE) algorithm by incorporating multiple mutation strategies and self-adaptive control parameters, thereby improving its search performance and adaptability to various problem landscapes. The iDE algorithm operates by employing a pool of mutation strategies, which are executed simultaneously during the mutation process. Each individual in the population is assigned a specific mutation strategy, and its success in generating better offspring determines the probability of that strategy being selected for future iterations. The iDE algorithm also adapts the control parameters, such as the scaling factor and crossover rate, according to the evolutionary process, enabling it to fine-tune its search behavior.

- **Particle Swarm Optimization (PSO)**

iDE is a robust and efficient optimization algorithm inspired by the social behavior of bird flocks and fish schools. PSO is a population-based, stochastic search technique particularly adept at solving continuous, non-linear, and non-convex optimization problems. The PSO algorithm operates by initializing a swarm of particles within the search space, with each particle representing a potential solution. The particles iteratively update their positions and velocities based on their personal best and the swarm's global best solution. The position updates incorporate both individual and social components, balancing exploration and exploitation. Each particle's velocity is updated by considering its inertia, cognitive component (representing the individual's experience), and social component (representing the swarm's collective experience). This velocity update rule enables the particles to search the solution space more effectively, converging towards the global optimum.

- **Artificial Bee Colony (ABC)**

ABC is a nature-inspired optimization algorithm developed to address complex optimization problems. The algorithm, based on the intelligent foraging behavior of honeybees, is a population-based search method that employs three types of bees: employed, onlooker, and scout bees. Employed bees exploit their associated food sources (solutions), while onlooker bees select food sources based on their fitness (quality). Scout bees explore the search space to discover new food sources. The interaction between these bee types facilitates a balance between exploration and exploitation, enhancing the search efficiency. Mernik et al. (2015) analyzed the algorithm's behavior and performance under different parameter settings, highlighting its robustness and adaptability in solving diverse optimization problems.

- **Non-dominated Sorting Genetic Algorithm 2 (NSGA2)**

NSGA2 is a prominent multi-objective optimization algorithm that builds upon its predecessor, NSGA, by introducing a fast elitist non-dominated sorting approach, enhanced diversity preservation, and reduced computational complexity.

This makes it more efficient and effective in solving multi-objective optimization problems. The NSGA2 algorithm operates by maintaining a population of candidate solutions, which evolve through genetic operators such as selection, crossover, and mutation. It employs a non-dominated sorting procedure to rank the solutions based on their objective function values, ensuring that multiple Pareto-optimal solutions are obtained. In addition to non-dominated sorting, NSGA2 utilizes a crowding distance metric to preserve diversity within the population, hence preventing premature convergence. Due to its efficiency, robustness, and ability to handle complex multi-objective problems, NSGA2 has become a popular choice for researchers and practitioners in various fields.

- **Multi-objective Evolutionary Algorithm by Decomposition (MOEA/D)**

MOEA/D is an innovative multi-objective optimization algorithm that employs a decomposition-based approach to effectively solve multi-objective optimization problems, transforming them into multiple scalar optimization subproblems, each one with an associated weight vector. In MOEA/D, the population of candidate solutions is evolved using genetic operators such as selection, crossover, and mutation. The algorithm utilizes a set of predefined weight vectors to decompose the multi-objective problem into multiple single-objective subproblems, which are then solved simultaneously. Solutions are updated according to a neighborhood concept, considering both their weighted objective values and proximity to other solutions in the decision space. The main strength of MOEA/D lies in its ability to efficiently generate diverse and high-quality Pareto-optimal solutions with more than two objectives.

- **Multi-objective Hypervolume-based Ant Colony Optimizer (MHACO)**

MGACO is a novel multi-objective optimization algorithm that combines the principles of Ant Colony Optimization (ACO) with the hypervolume indicator, a widely used performance metric in multi-objective optimization, to efficiently find diverse and high-quality Pareto-optimal solutions.

MHACO operates by adapting the traditional ACO framework to handle multi-objective problems. The algorithm employs artificial ants to construct solutions by traversing the search space, guided by pheromone trails and heuristic information. The hypervolume indicator is utilized to measure the quality of solutions and update pheromone trails, promoting the exploration of the solution space in areas with higher hypervolume contributions.

- **Non-dominated Sorting PSO (NSPSO)**

NSPSO is an advanced multi-objective optimization algorithm which combines the Particle Swarm Optimization (PSO) framework with the non-dominated sorting strategy to effectively solve multi-objective optimization problems. NSPSO inherits the robustness and simplicity of the original PSO, while extending its capabilities to handle multiple conflicting objectives. In NSPSO, a swarm of particles is evolved iteratively through position and velocity updates, similar to the traditional PSO. The main innovation lies in the integration of non-dominated sorting to rank the particles based on their objective function values, ensuring that multiple Pareto-optimal solutions are obtained. To maintain diversity among solutions, NSPSO introduces a crowding distance metric, preventing premature convergence.

All these algorithms inherit from the parent class `Algorithm` which represents a common interface to all optimization algorithms. All implemented algorithms must implement a `evolve()` method that takes as input a `population` object and returns a new one generated by the evolution of the original.

e2doptimization module implements a factory method to create `problem` objects. The class `OptimizationProblem` represents an optimization problem that must include at least two methods: `fitness()` and `get_bounds()`. The first one takes as parameter the decision vector and returns the optimization objectives and constraints results. The second returns a tuple with the lower bounds vector and the upper bounds vector, representing the boundaries of the decision vector elements. If constrains are defined in the `fitness()` method, then two additional methods are needed: `get_nic()` that returns the number of inequality constrains and `get_nec()` that returns the number of equality constraints. For multi-objective optimization problems, an additional method must be defined, `get_nobj()` that returns the number of objectives.

Table 5. List of available algorithms in eco2des.

Algorithm	Capabilities	Source
Extended Ant Colony Optimization (GACO)	Single objective Constrained or unconstrained Integer programming	(Schlüter, Egea, and Banga 2009)
Differential Evolution (DE)	Single objective Unconstrained	(Price, Storn, and Lampinen 2005)
Self-adaptive DE (iDE)	Single objective Unconstrained	(Elsayed, Sarker, and Essam 2011)
Particle Swarm Optimization (PSO)	Single objective Unconstrained	(Kennedy and Eberhart 1995)
Artificial Bee Colony (ABC)	Single objective Unconstrained	(Mernik et al. 2015)
Non-dominated Sorting Genetic Algorithm 2 (NSGA2)	Multi-objective Unconstrained Integer programming	(Kalyanmoy Deb et al. 2000)
Multi-objective Evolutionary Algorithm by Decomposition (MOEAD)	Multi-objective Unconstrained	(Zhang and Li 2007)
Multi-objective Hypervolume-based Ant Colony Optimizer (MHACO)	Multi-objective Unconstrained	(Acciarini, Izzo, and Mooij 2020)
Non-dominated Sorting PSO (NSPSO)	Multi-objective Unconstrained	(X. Li 2003)

To conclude with the main classes, the class `Population` represents a population of individuals that are potential candidate solutions to a given optimization problem. In e2doptimization, as in pygmo, an individual is determined as follows:

- by a unique ID used to track the individual across generations and migrations,
- by a decision vector,
- by the fitness evaluated by a `problem` object, including objectives and equality and inequality constraints if present.

Finally, as e2dlca and e2dlcc modules, e2doptimization includes functionalities to support the life cycle interpretation phase. Hence, this module is able to plot the Pareto front after solving an optimization problem (Figure 38), as well as to export its points to Excel including the decision vector, objectives and constraints values.

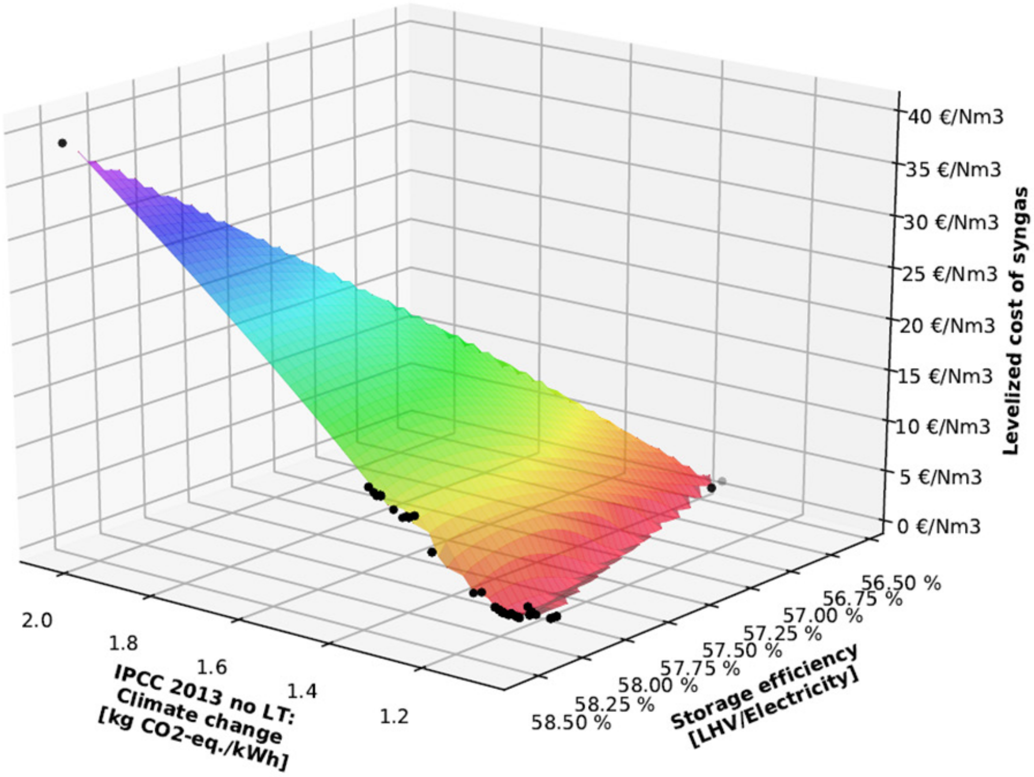

Figure 38. Pareto front example from eco2des.

7. CASE STUDIES

7.1. Introduction

In this section two case studies are presented that were used during the development of the thesis to test, validate and improve both, the presented methodology for the eco-design of industrial processes, and the eco2des tool.

The first case study is the carbon dioxide methanation for wind energy storage in the natural gas grid. This case study is used to present the features of eco2des, as well as a user guide on how to apply the tool for the eco-design of an industrial process.

The second case study is about a production plant of synthetic fuels from biomass. In this case, the objective is to present a more complex project in a controversial technology which is under study to decarbonize the industrial sector. Therefore, the capabilities of eco2des for providing sustainable designs and reliable insights on the technology under study is proved.

Furthermore, it is worth to mention that both the methodology and the tool were also validated with additional case studies which cannot be disclosed as they are protected under the industrial property of either Contactica S.L. (the company involved in the industrial PhD project) or any of its customers.

7.2. CO_2 methanation for wind energy storage in the natural gas grid

7.2.1. Background

Currently, conventional energy sources such as nuclear power or fossil fuels are being replaced by renewable ones such as wind or solar energy. However, most of the renewable sources cannot provide a base load electric power. To overcome this problem, storage systems have to be integrated in the power grid. For seasonal storage of the energy (charge / discharge period from 1 day to 1 year) in huge capacities, electrical energy can be converted into chemical energy by transferring it into fuels. The logical pathway is the conversion of electrical energy into hydrogen by water electrolysis, but nowadays there is no a hydrogen grid, or a large enough storage system developed in any country. Until this requirement is satisfied, the highly developed natural gas grids can be used for the transport of excess energy (Bassano et al. 2019), using electrolysis to produce hydrogen to react with carbon dioxide in a methanation synthesis to produce synthetic natural gas (SNG). Therefore, in addition to providing an energy carrier, the process consumes carbon dioxide, contributing to the reduction of greenhouse gas emissions (GHGE).

The methanation reactions of carbon monoxide and carbon dioxide were discovered at the beginning of the 20th century by (Sabatier and Senderens 1902). The methanation of carbon dioxide is an exothermic catalytic reaction and is typically operated at temperatures between 200°C and 550°C depending on the used catalyst:

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O \qquad \Delta H_R^0 = -252\ \frac{kJ}{mol}$$

7.2.2. Goal and scope definition

The goal of this study is to demonstrate the potential of the eco2des tool. Consequently, the sustainability-based optimization of the current case study is carried out using a life cycle perspective, minimizing both environmental and economic impacts.

The evaluated foreground system is shown in Figure 39, which covers the supply of carbon dioxide from an industrial source, the supply of hydrogen from the electrolysis of excess wind energy into the methanation process and the production of synthetic natural gas (SNG) for seasonal storage. The plant has the capacity to produce 356 kg/h of hydrogen, but due to the variability of the excess energy produced a capacity factor of 50 % was assumed. For the background system in the LCA, the ecoinvent 3.6 version (Wernet et al. 2016) with the Cut-Off system model is used to model the value chain.

A cradle-to-gate approach was chosen for the system boundaries. Since the optimization was made over process design parameters, this approach was considered sufficient. Therefore, the emissions upon combustion of the SNG were chosen to fall out of the scope of the assessment, since this fuel is not compared with conventional natural gas or other alternatives, but with other process alternatives during the optimization.

Finally, the functional unit (FU) of the product system is 1 Nm^3 of SNG. According to it, the global warming (GW) environmental impact category was selected to evaluate the environmental performance of the process. Furthermore, this study uses present worth method to compute capital expenditure (CAPEX) and operational expenditure (OPEX) over the whole life cycle of the plant not considering externalities. The cost of principal components of the plant were taken from the literature. Finally, levelized cost of production (LCOP) of SNG, in €/Nm^3, was computed as a measure of economic performance.

7.2.2.1. Problem statement

Given:

- A process superstructure of potential topological and operational alternatives of the CO_2 methanation for wind energy storage in the natural gas grid, based on its simulation defined by thermodynamics and kinetics relationships, and mass and energy balances.
- A lifetime, the price of the final products, the cost of the equipment, raw materials and utilities.
- The environmental burdens of the upstream activities of the value chain.

The problem then consists of optimizing the production process using its operational variables, minimizing the environmental impacts and costs, and maximizing the storage efficiency of the system.

7.2.3. Predictive life cycle inventory analysis

7.2.3.1. Process simulation

Figure 39 illustrates the layout of the Aspen Plus simulation. For the determination of the optimal reactor concept, the kinetic model 12 of (Kopyscinski 2010) was used. The rate equations follow the Langmuir-Hinshelwood approach for the proposed two-step reaction mechanisms.

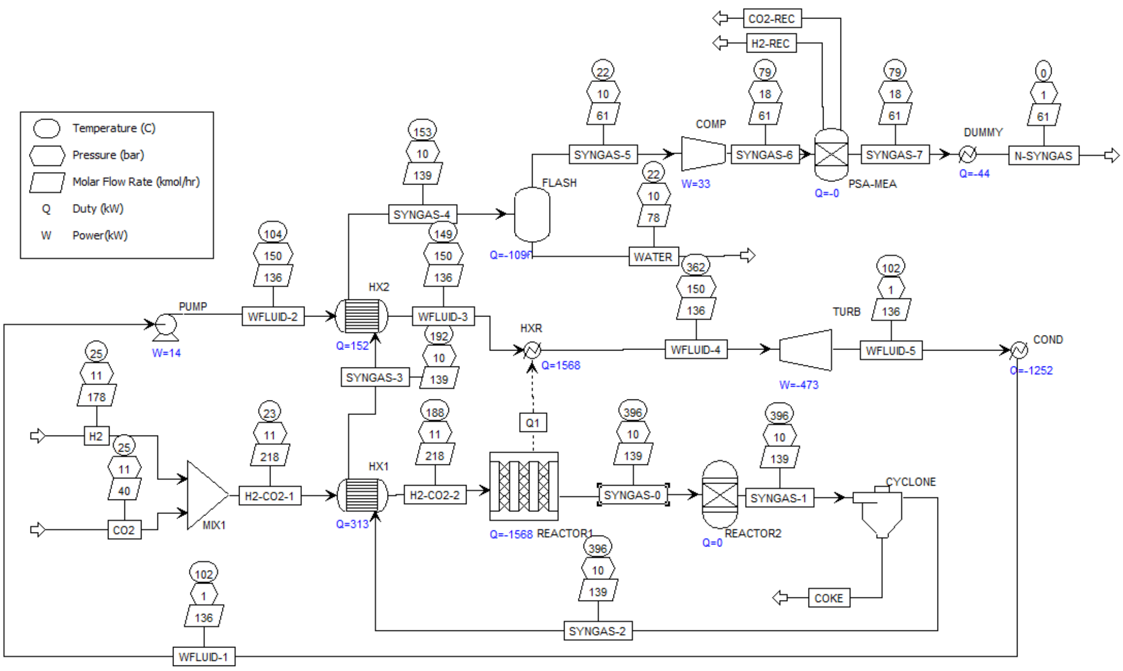

Figure 39. Aspen Plus flowsheet of the CO_2 methanation process simulation

In the first step, carbon dioxide and hydrogen are converted to carbon monoxide and water via the water-gas shift reaction:

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H_R^0 = -165\ \frac{kJ}{mol}$$

In the subsequent reaction, methane is formed from carbon monoxide and hydrogen:

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \qquad \Delta H_R^0 = -206\ \frac{kJ}{mol}$$

The rate equations for the methanation and water gas shift reaction from Kopyscinski model 12 are, respectively:

$$r_1 = \frac{k_1 \cdot K_C \cdot p_{CO}^{0.5} \cdot p_{H_2}^{0.5}}{\left(1 + K_C \cdot p_{CO} + K_{OH} \cdot p_{H_2O} \cdot p_{H_2}^{-0.5}\right)^2}$$

$$r_2 = \frac{k_2 \cdot \left(K_\alpha \cdot p_{CO} \cdot p_{H_2O} - \frac{p_{CO_2} \cdot p_{H_2}}{K_{eq}}\right)}{p_{H_2}^{0.5} \cdot \left(1 + K_C \cdot p_{CO} + K_{OH} \cdot p_{H_2O} \cdot p_{H_2}^{-0.5}\right)^2}$$

Where:

- k_i is the rate constant for the reaction i.
- K_j is the adsorption equilibrium constant for the substance j.
- p_j is the partial pressure of substance j.
- K_α is the adsorption equilibrium constant for the active sites of the catalyst where the reaction takes place.
- K_{eq} is the equilibrium constant for the reaction, indicating the ratio of product to reactant partial pressures at equilibrium.

The model parameters were implemented into a RPLUG reactor of Aspen Plus (REACTOR1 in Figure 39). Furthermore, the resulted gases are connected to a RGIBSS reactor to minimize the free energy of Gibbs following the Boudouard reaction (Basu 2018):

$$2CO \leftrightarrow C + CO_2 \qquad \Delta H_R^0 = -172\ \frac{kJ}{mol}$$

This way the potential formation of coke is measured and considered for solid deposition over the catalyst, and, hence, the environmental and economic models would consider the regeneration and replacement cycles of it. The heat of the gas stream is recovered in the inlet stream of the reactor as well as in the hybridization with a Rankine cycle to generate electricity, which operates with water or cyclopentane as working fluid (it is a decision variable). Finally, the gas is dried and compressed to be injected into the grid. A dummy heater is introduced in the simulation to evaluate the composition of the SNG at normal conditions (0 °C, 1.1325 bar). Then, following the Spanish regulation (Ministerio para la Transición Ecológica 2018), if the hydrogen molar concentration is higher than a 5 % a pressure swing adsorption, PSA, unit is needed, recovering 90 % of the hydrogen which is recirculated. Moreover, if carbon dioxide molar concentration is higher than a 2 % a monoethanolamine (MEA)-based capture is needed, recovering 97% of the carbon dioxide which is then recirculated. Both of them are modelled as black boxes, taking the processes conditions, raw materials and utilities from (Susmozas, Ana 2015) for the PSA unit and from (Ferrara et al. 2017) for the MEA-based capture. Table 6 shows the correlations taken from literature and introduced in the simulation through Aspen Plus Calculators.

Table 6. PSA and MEA-based capture raw materials and utilities.

PSA electricity utility [kW]	$0.029 \cdot SNG\_flow[Nm^3]$
MEA makeup $\left[{}^{kg}/_{h}\right]$	$0.7624 \cdot CO_2\_recirculated \left[{}^{kg}/_{h}\right]$
$MEA\ capture\ duty\ utiliy\ [kW]$	$1.42 \cdot CO_2\_recirculated \left[{}^{kg}/_{h}\right]$
$MEA\ capture\ electricity\ utiliy\ [kW]$	$0.18 \cdot CO_2\_recirculated \left[{}^{kg}/_{h}\right]$
$MEA\ capture\ cooling\ water\ \left[{}^{kg}/_{h}\right]$	$349.3 \cdot CO_2\_recirculated \left[{}^{kg}/_{h}\right]$

In order to start taking advantages of the capabilities of eco2des, first, a new project needs to be defined and the CO_2 methanation process simulation linked to it. The Python code in Figure 40 illustrates that.

Once the simulation is loaded, the whole data from it may be accessed through the object `e2d.project.simulation` as it will be presented afterwards.

```python
import eco2des as e2d

e2d.projects.create_project(
    name="CO2 methanation for energy storage",
    reference_currency="EUR",
    year=2020,
    location="ES",
)
e2d.projects.current = "CO2 methanation for energy storage"
e2d.project.simulation.load_simulation(".//Sabatier_k.bkp")
```

Figure 40. Create new project and load simulation file in eco2des.

7.2.3.2. Environmental Inventory

eco2des allows the user to link the activities of the LCA model with values directly taken from the Aspen Plus simulation outputs generating a predictive environmental inventory. This approach eases the development of studies in optimization, scale-up, sensitivity analysis or stochastic calculations of uncertainty from an environmental perspective. Hence, the current approach increases the productivity of experts, due to the construction of variable and automated inventories linked to the results from the simulation in each evaluation step.

In order to do that, first, an activity must be created for the `“CO2 methanation for energy storage”` project using the `create_activity()` method from e2dlca (Figure 41).

This method creates an activity given a name and a production amount, additional parameters may be defined as the code illustrates in Figure 41. This activity is stored in a SQL database related to the working-on project. Then, this activity must be populated with inventory data. First, data regarding background processes were taken from ecoinvent 3 database (Wernet et al. 2016), building the technosphere (i.e. manufactured goods and services) inventory calculated per FU of the system. ecoinvent 3 database can be integrated into eco2des if the user has a license using the credentials to download it or importing it from a local path. Once the database is imported, the user is able to point to it with an object (see Figure 42).

```
e2d.project.lca.create_activity(
    name="Sabatier for renewable energy storage",
    location="ES",
    unit="normal cubic meter",
    ref_product="SNG",
    production_amount=1.0,
)

sabatier = e2d.project.lca.activities["Sabatier for renewable energy storage"]

```

Figure 41. Create product system in eco2des.

```
ei36 = e2d.lca.database('Ecoinvent 3.6 cut-off')

```

Figure 42. Pick an environmental background database in eco2des.

For this case study, the ecoinvent 3.6 version with the Cut-Off system model is used. The following code in Figure 43 illustrates how to populate the main activity of the project with technosphere activities from the ecoinvent 3 database.

First, a function is created to compute the amount of the activity which is added to the life cycle inventory in line 1. This function is executed in each evaluation of the optimization population, generating a new amount of this particular exchange depending on the new results provided by the simulation. Hence, a predictive and automated inventory is created.

```python
1  def lci_wind_energy():
2
3      hydrogen_in = e2d.project.simulation.streams["H2"]
4      hydrogen_in_mass_flow, _ = hydrogen_in.output.total_mass_flow()
5      hydrogen_rec = e2d.project.simulation.streams["H2-REC"]
6      hydrogen_rec_mass_flow, _ = hydrogen_rec.output.total_mass_flow()
7      hydrogen_mass_flow = hydrogen_in_mass_flow - hydrogen_rec_mass_flow
8
9      electricity, _ = e2d.project.simulation.utilities["ELECTRICITY"].total_value
10
11     sng = e2d.project.simulation.streams["N-SYNGAS"]
12     sng_volume_flow, _ = sng.output.total_volume_flow()
13
14     return (49 * hydrogen_mass_flow + electricity) / sng_volume_flow
15
16
17 wind_energy = [
18     act
19     for act in ei36
20     if act["name"] == "electricity production, wind, >3MW turbine, onshore"
21     and act["location"] == "ES"
22 ][0]
23
24 sabatier.new_exchange(amount=lci_wind_energy, input=wind_energy, type="technosphere")
25 sabatier.save()
26
```

Figure 43. Add a technosphere exchange to the product system in eco2des.

In this function, the capabilities of e2dsimulation are shown to extract simulation data:

1. The H2 stream (Figure 39) is selected in line 3, returning a `MaterialStream` object.
2. The total mass flow of this stream is retrieved in line 4. This method returns a tuple with the actual value selected and a string representing the unit defined in the simulation.
3. The H2-REC stream (Figure 39) is selected in line 5, returning a `MaterialStream` object.
4. The total mass flow of this stream is retrieved in line 6.
5. The hydrogen input is calculated by subtracting the recovered hydrogen from the fresh one in line 7.
6. The total electricity utility is read from the simulation in line 9.
7. The N-SYNGAS stream (Figure 39) is selected in line 11, returning a `MaterialStream` object.
8. The total volume flow of this stream is read in line 12.

9. Finally, in line 14 the amount of electricity produced from the wind turbine per FU is returned.

Then, from line 17 to 22, a list comprehension is used to choose the technosphere activity to be linked from the ecoinvent 3 database. After, this activity is introduced as a new exchange into the reference project activity (aka product system) using the `new_exchange()` method in line 24, which takes as parameters the activity from a LCI database, the amount, which could be a callable that will be executed to get the actual numeric value of the exchange; and the type of exchange which could be "production" for the reference product of the product system, "technosphere" for exchanges coming from the technology matrix, or "biosphere" for elementary flow exchanges coming from the biosphere matrix. Finally, in order to actually apply this changes in the product system activity and persist them in the database the `save()` method needs to be called in line 25.

This procedure has to be replicated for each technosphere activity linked to the project in order to cover the whole value chain of the LCA model. Table 7 shows the technosphere inventory used in this case study, where $H_{2,in}$ is the mass flow of hydrogen from electrolysis (linked to the inventory directly from simulation data as Figure 43 shows). Then, $electricity$ is the surplus of electricity produced by the Rankine Cycle of the process which is modeled as it is consumed by the electrolyzer to produce hydrogen. $CO_{2,\,rec}$ is the amount of carbon dioxide recirculated if a MEA-based capture is needed, catalyst is the catalyst load for the methanation reactor, $f_{capacity}$ is the capacity factor of the plant, $working_{fluid}$ is the amount of working fluid required in the Rankine cycle which could be water or cyclopentane depending on the chosen decision variable. Finally, $wastewater$ is the water flow from the SNG drying process.

Correlations for activities regarding electrolyzed hydrogen (items 1, 2 y 3 in Table 7) were taken from (Valente et al. 2020) and adapted to the FU of the product system case study. The amount of market for monoethanolamine activity is modelled following the correlation presented in Table 6 for the MEA makeup. The catalyst load is computed multiplying the methanation reactor volume (taken from Aspen Plus simulation data) by the catalyst density, 1500 kg/m^3, and by one minus the catalyst void ratio, 0.6, as (Moioli, Gallandat, and Züttel 2019) published for Ru/Al2O3 used in this process. Moreover, catalyst composition was also taken from this study. Since the ruthenium market or production are not integrated in ecoinvent version 3.6, this activity was modelled as market for rhodium, as this activity has really close environmental impacts (Nuss and Eckelman 2014). For the working fluid of the Rankine cycle, a 1 % of makeup is assumed. Furthermore, if the fluid chosen is cyclopentane their environmental burden is modeled as a 50 % of the environmental impacts of fraction 1 of naphtha separation which is a mixture of cyclopentane and 2,2-dimethylbutane. Finally, carbon dioxide input is considered free of environmental burdens, since it is a waste from the capture process of an industrial source.

Table 7. Technosphere inventory data of the CO_2 methanation process for energy storage (FU: 1 Nm3 of SNG)

Activity name	Amount	Unit
electricity production, wind, >3MW turbine, onshore, ES	$\frac{49 \cdot H_{2,in} + electricity}{SNG}$	kWh
market for water, deionized, Europe without Switzerland	$\frac{11{,}2 \cdot H_{2,in}}{SNG}$	kg
market for potassium hydroxide, GLO	$\frac{0{,}85 \cdot H_{2,in}}{SNG}$	kg
market for monoethanolamine, GLO	$\frac{0.7624 \cdot CO_{2,rec}}{SNG}$	kg
market for rhodium, GLO	$\frac{catalyst \cdot 0{,}5\%}{SNG} \cdot \frac{1}{3/f_{capacity}}$	kg
market for aluminium oxide, non-metallurgical, IAI Area, EU27 & EFTA	$\frac{catalyst \cdot 99{,}5\%}{SNG} \cdot \frac{1}{3/f_{capacity}}$	kg
fraction 1 from naphtha separation to generic market for chemical, organic, GLO	$\frac{0{,}5 \cdot working_{fluid} \cdot 1\%}{SNG}$	kg
market for water, decarbonized, ES	$\frac{working_{fluid} \cdot 1\%}{SNG}$	kg
water production, completely softened, RER	$\frac{working_{fluid} \cdot 1\%}{SNG}$	kg
market for wastewater, from residence, RoW	$\frac{wastewater}{SNG}$	m3

Once the technosphere inventory is built, the biosphere inventory of the product system has to be populated. For this purpose, following the Brightway2 convention, the biosphere3 database is used. This database has all the resource and emission flows from the ecoinvent database. The code in Figure 44 illustrates how to populate the product system activity with a biosphere flow:

```
1  bio = e2d.lca.database("biosphere3")
2
3
4  def lci_co2():
5
6      coke = e2d.project.simulation.streams["COKE"]
7      coke_mass_flow, _ = coke.output.total_mass_flow()
8
9      sng = e2d.project.simulation.streams["N-SYNGAS"]
10     sng_volume_flow, _ = sng.output.total_volume_flow()
11
12     return 44.01 / 12 * coke / sng
13
14
15 co2 = [
16     exc
17     for exc in bio
18     if "Carbon dioxide, fossil" in exc["name"]
19     and "non-urban air or from high stacks" in exc["categories"]
20 ][0]
21
22 sabatier.new_exchange(amount=lci_co2, input=co2, type="biosphere")
23 sabatier.save()
24
```

Figure 44. Add a biosphere exchange to the product system in eco2des.

First, the biosphere3 database is selected in line 1. Then, a function to compute the amount of carbon dioxide emitted to the air is defined in lines 4 to 12. This function takes the amount of coke generated in the process from the Aspen Plus simulation and use it to compute the carbon dioxide, as the LCA model assumed that the catalyst regeneration is done through a thermal process which combusts the deposited coke following the next reaction:

$$C + O_2 \rightarrow CO_2$$

Then, from lines 15 to 20, a list comprehension is used to choose the biosphere exchange to be linked from the biosphere3 database. Finally, this exchange is introduced into the project activity using the `new_exchange()` method as explained before. Following this procedure, the biosphere inventory is built. Table 8 shows the biosphere inventory for this case study, where $water_{utility}$ is the cooling water needed in the Rankine cycle whose value is taken from the simulation assuming a 0.5 % of losses. It is modelled as water from unspecified natural origin. Finally, $coke$ is the amount of coke generated in the methanation reactor which produces carbon dioxide and takes oxygen as natural resource when it is combusted in the regeneration cycle.

Table 8. Biosphere inventory data of the CO_2 methanation process for energy storage (FU: 1 Nm3 of SNG)

Elementary flow	Amount	Unit
Water, cooling, unspecified natural origin	$\frac{water_{utility} \cdot 0.5\ \%}{SNG}$	m3
Carbon dioxide, fossil, to non-urban air or from high stacks	$\frac{44{,}01/_{12} \cdot coke}{SNG}$	kg
Oxygen, to in air	$\frac{44{,}01/_{32} \cdot coke}{SNG}$	kg

7.2.3.3. Economic inventory

CAPEX estimation

CAPEX was calculated in the eco2des framework applying the factored estimation method (Towler and Sinnott 2013a) for the main equipment pieces. The cost of principal components of the plant were computed using the built-in correlations of eco2des and scaling factors for the equipment in Table 9 using equation 6.

Table 9. Basic costs for major equipment with scaling factors

Equipment	Reference capacity	Reference cost, €	Scale factor	Reference
Electrolysis	1 kWe	175	1	(U.S. Department of Energy 2015)
PSA unit	155.24 tonne/day (H_2)	7,319,000	0.7	(Susmozas, Ana 2015)
MEA-based CO_2 capture	3.9 Nm3/s (raw gas)	5,190,000	0.7	(Holmgren 2015)

The following code in Figure 46 and Figure 47 exemplifies how to add equipment cost to the project in the eco2des framework which are linked to the simulation results, creating the predictive economic inventory. As example, electrolysis and methanation reactor (modeled with the vessel built-in correlation) are shown.

```
1  capex = e2d.project.lcc.capex
2
3
4  def lcc_kW_electrolyzer():
5
6      hydrogen_in = e2d.project.simulation.streams["H2"]
7      hydrogen_in_mass_flow, _ = hydrogen_in.output.total_mass_flow()
8      hydrogen_rec = e2d.project.simulation.streams["H2-REC"]
9      hydrogen_rec_mass_flow, _ = hydrogen_rec.output.total_mass_flow()
10     hydrogen_mass_flow = hydrogen_in_mass_flow - hydrogen_rec_mass_flow
11
12     return hydrogen_mass_flow * 44.7
13
14
15 capex.add_scaled_equipment(
16     name="Electrolyzer",
17     capacity=lcc_kW_electrolyzer,
18     reference_capacity=1,
19     reference_cost=175,
20     scaling_factor=1,
21     process_type="Fluids",
22     year=2015,
23 )
24
```

Figure 45. Add equipment to the LCC model estimated by a scaling method in eco2des.

First, the `capex` object is stored in a variable (line 1) to simplify subsequent code. Then, a function is defined from line 4 to 12 which extracts the mass flow of hydrogen produced in the electrolyzer and estimates the electrolyzer power capacity by assuming an electrolysis efficiency of 75 %. In these conditions, 1 kg of hydrogen needs 44.7 kWh of energy to be produced (U.S. Department of Energy 2015).

Then, a new equipment estimation is added to the `capex` object using the factory method `add_scaled_equipment()`, from line 15 to 23. This method takes as parameters the name of the equipment (this could be used as key to access the equipment in `capex.equipments` mapping object), a callable that computes the capacity of the equipment, the reference capacity, the reference cost, the scaling factor, the process type (it is a literal variable which could be "Fluids", "Fluids-Solids" or "Solids" that is used to get the appropriate factors to estimate the equipment erection costs) and the year of the reference cost which is used to apply cost escalation to the year defined in the project.

```python
def lcc_sabatier_flow():
    stream_in = e2d.project.simulation.streams["H2-CO2-2"]
    vol_flow, _ = stream_in.output.total_volume_flow()
    return vol_flow


def lcc_sabatier_rt():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    residence_time, _ = rplug.output.residence_time()
    return residence_time


def lcc_sabatier_ld():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    length, _ = rplug.output.length()
    diameter, _ = rplug.output.diameter()
    return length / diameter


def lcc_sabatier_pres():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    pressure, _ = rplug.output.pressure_max()
    return pressure


def lcc_sabatier_temp():
    rplug = e2d.project.simulation.blocks["REACTOR1"]
    temperature, _ = rplug.output.temperature_max()
    return temperature


capex.add_vessel(
    name="Methanation reactor",
    volume_flow=lcc_sabatier_flow,
    residence_time=lcc_sabatier_rt,
    length_diameter_ratio=lcc_sabatier_ld,
    pressure=lcc_sabatier_pres,
    temperature=lcc_sabatier_temp,
    vessel_kind="horizontal",
    material="Stainless 304",
    process_type="Fluids",
)
```

Figure 46. Add equipment to the LCC model estimated by a built-in correlation in eco2des.

In Figure 47, the methanation reactor cost is modeled using the eco2des built-in correlation for a vessel. This correlation uses the method detailed in the rules for constructing pressure vessels from the American Society of Mechanical Engineers (ASME 2017) to calculate the amount of material needed depending on the operational conditions and, consequently, estimates the vessel cost. In order to do so, the factory method `add_vessel()` is used from line 32 to line 42. This method needs 5 parameters that are taken from the Aspen Plus simulation file:

1. The volumetric flow that is read from the H2-CO2-2 stream (Figure 39), as represented in lines 1 to 4 in Figure 47.
2. The reactor residence time, which is extracted in the function defined from line 7 to line 10.
3. The length to diameter ratio of the reactor. This data is computed in function `lcc_sabatier_ld()` in lines 13 to 17, using e2dsimulation capacities to read both the length and the diameter of the RPlug reactor.
4. The maximum pressure which is extracted from the simulation output in the function defined in lines 20 to 23.
5. The maximum temperature which is also extracted from the simulation output in the function defined in lines 26 to 29.

Likewise, the other plant equipment is introduced in the framework. Equipment from Table 9 is estimated in eco2des as the electrolyzer and the other equipment in the flowsheet with built-in correlations. These are: a storage tank, heat exchangers, a pump, a steam turbine and a compressor.

To conclude, catalysts have a special treatment inside eco2des framework, because the first load is capitalized and the rest during the plant lifetime are considered as operational expenditure. Ru/Al_2O_3 cost is estimated to be double the costs of the raw materials. Ruthenium and alumina costs were taken from (Glacier Media Group 2020) and (The London Metal Exchange - an HKEX Company 2020), respectively.

OPEX estimation

OPEX estimation is performed in eco2des frameworks as detailed in Section 6.4.4. The following code in Figure 48 illustrates how the `opex` object is populated with some inputs that the user must define, many of them linked to the simulation model.

```
1  opex = e2d.project.lcc.opex
2
3  opex.operating_labour(
4      positions=4, employees=4.8, salary=30000, interannual_variance=0.015
5  )
6
7  opex.loan(percent=0.6, interest=0.04, years=10)
8
9  opex.depreciation(type="linear", value=0.07, residual_value=0)
10
11
12 def lcc_co2():
13
14     co2_in = e2d.project.simulation.streams["CO2"]
15     co2_in_mass_flow, _ = co2_in.output.total_mass_flow()
16     co2_rec = e2d.project.simulation.streams["CO2-REC"]
17     co2_rec_mass_flow, _ = co2_rec.output.total_mass_flow()
18     co2_mass_flow = co2_in_mass_flow - co2_rec_mass_flow
19
20     f = e2d.project.capacity_factor()
21
22     return co2_mass_flow / 1000 * f * 8760
23
24
25 opex.add_raw_material(
26     name="CO2", quantity=lcc_co2, price=10, interannual_variance=0.015, unit="Tn"
27 )
28
```

Figure 47. Add OPEX costs in eco2des.

First, the `opex` object is stored in a variable in line 1. Then, operating labour cost is estimated from the number of the job positions needed in the plant, the number of full-time employees (FTE) needed to cover one position and the average salary. In this case study, 4 positions with 4.8 FTE each and an average salary of 30,000 € were assumed. Furthermore, an interannual variance is included that will increase the labour costs each year in the lifetime of the project. In line 7, the `loan()` method is used to include the external resources in the project. This method needs the percentage of the CAPEX that is covered with a loan, the interest rate and the years in which the loan will be returned. Therefore, the LCC model assumed a financial scheme of 40 % own resources and 60 %

borrowed resources, with a loan with a 4 % of interest rate and ten years period. In line 9, the depreciation costs are included in the model. A linear depreciation model with a value of 7 % per year and without any residual value at the end of the project was considered. Finally, as an example, the code illustrates how to add a raw material cost to the model. Hence, a function is defined from lines 12 to 22 to extract data from the simulation to compute the tonnes of carbon dioxide that are fed into the methanation plant during a year. This function is linked to the LCC model using the `add_raw_material()` factory method in lines 25 to 27. The parameters of this function are the raw material name which will be used as key to get raw material in the `opex.raw_materials` object, the quantity which is the callable to extract the value from the simulation or just a number input, the price of the raw material, the unit of measure for the quantity and the interannual variance of the price to be considered by the LCC model. Similarly, the `add_utility()` factory method may be used to add utility costs. Notice that some OPEX methods receive an optional argument called `interannual_variance`. It is used in the following LCC model resolution to add annually a percentual increment (or decrement) in the OPEX item. In this case study, sale prices, salaries and raw materials have an annual variance of 1.5 %; maintenance of 2.5 % and utilities of 2 %.

To conclude, the rest of raw materials and utilities are defined alike the carbon dioxide in the previous Figure 48. Their prices may be checked in Table 10.

Table 10. Raw materials and utilities prices

Raw material / utility	Cost, €
Carbon dioxide, 1 tonne	10
Water (working fluid), 1 tonne	1.29
Cyclopentane (working fluid), 1 tonne	1000
MEA, 1 tonne	1100
KOH, 1 tonne	550
Deionized water, 1 tonne	0.88
Refrigeration water, 1 tonne	0.027

For carbon dioxide, only transport cost was considered assuming that the capture process is out of the system boundaries. This price is taken from (McCoy and Rubin

2005). Furthermore, the replacement of the electrolyzer cells is defined inside the framework at a cost of 25 % of total purchased capital every 7 years (National Renewable Energy Laboratory (NREL) 2012).

7.2.4. Life cycle impact assessment

7.2.4.1. Environmental impact assessment

Global warming (GW) environmental impact category was selected to evaluate the environmental performance of the process. It was computed using the global warming potentials of the IPCC 2013 method (Stocker et al. 2013) without long term emissions. The code in Figure 45 shows how the impact assessment phase is carried out in eco2des.

```
1 sabatier = e2d.project.lca.activities["Sabatier for renewable energy storage"]
2
3 ipcc = ("IPCC 2013 no LT", "climate change", "GWP 100a")
4
5 e2d.project.lca.LCA({sabatier: 1}, method=ipcc)
6
```

Figure 48. Impact assessment phase in eco2des.

In line 1, the product system activity is selected. Then, in line 3, an impact assessment method is chosen. Following Brightway2 standards, a method is defined as a tuple. The user may list all the available methods in the tool running the following line of code `list(e2d.lca.methods)`. Then, the LCA model is defined calling the `LCA()` method from e2dlca giving as arguments a dictionary containing the reference activity and the functional unit amount; and the LCIA method (see line 5 in Figure 45).

7.2.4.2. Economic impact assessment

LCOP was selected to evaluate the economic performance of the process. In the present worth method, it is essential to determine a discount rate to find the equivalent value for each alternative in a common base date. In this study, a nominal discount rate of 10 % was used to compute the LCOP of the SNG, assuming a plant lifetime of 30 years and a construction period of 1.5 years. This discount rate is assumed to be the expected profitability by the plant investors. Figure 49 illustrates how to add these model inputs to the LCC model in eco2des.

```
e2d.project.lcc.cash_flow(years=30, discount_rate=0.1, construction_time=1.5)
```

Figure 49. Add cash flow model inputs in eco2des.

7.2.5. Multi-objective optimization

As abovementioned, the main goal of this study is to demonstrate the potential of eco2des framework for optimizing the economic and environmental performance of the case study without compromising main technical parameters.

Therefore, a first optimization problem with three objectives has been built to minimize global warming (GW) impact, LCOP of SNG and maximize the system storage efficiency ($\eta_{storage}$) measured as the lower heating value (LHV) of the SNG produced, divided by the electricity used (wind power for electrolysis minus the generated power in the Rankine Cycle).

The resolution of this problem shows that environmental and economic objectives are non-conflicting in this case study. So, a second optimization problem has been proposed with two objectives: minimizing LCOP of SNG and maximizing storage efficiency. Both multi-objective optimization problems (MOOP) share three constraints and five decision variables detailed in Table 11 and whose bounds were chosen by preliminary sensitivity analysis.

Table 11. MOOPs formulation

Objective functions		
MOOP1	$Min\left(GW, LCOP, -\eta_{storage}\right)$	
MOOP2	$Min\left(LCOP, -\eta_{storage}\right)$	
Subject to		
Constraint 1	$SNG[H_2] < 5\ \%$	
Constraint 2	$SNG[CO] < 2\ \%$	
Constraint 3	$SNG[CO_2] < 2\ \%$	
Decision variables	**Lower bound**	**Upper bound**
H_2/CO_2 ratio	4	5
Reactor temperature, C	250	400
Reactor length, m	1	20
Reactor LD ratio	1	10
Working fluid (integer)	0	1

$SNG[H_2]$: H_2 molar composition in SNG; $SNG[CO]$: CO molar composition in SNG; $SNG[CO_2]$: CO_2 molar composition in SNG; LD: length to diameter

For solving quickly multi-objective optimization problems finding reasonable solutions, eco2des offers a set of different genetic algorithms. In this case study, multi-objective evolutionary algorithm with decomposition, MOEA/D, (Zhang and Li 2007) was selected for MOOP1; and non-dominated sorting genetic algorithm II, NSGA-II, (K. Deb et al. 2002) for MOOP2. Constraints were integrated following the death penalty method (Back 1991), in which infeasible individuals are rejected in the selection procedure regardless their level of infeasibility.

With illustrative purpose, the following figures shows how to formulate and solve MOOP1 using eco2des. First, objectives must be defined as Figure 50 shows.

```python
1  def has_passed_constraints():
2      sng = e2d.project.simulation.streams["N-SYNGAS"]
3
4      sng_h2 = sng.composition["H2"].output.mole_frac()
5      sng_co = sng.composition["CO"].output.mole_frac()
6      sng_co2 = sng.composition["CO2"].output.mole_frac()
7
8      if sng_h2 > 0.05 or sng_co > 0.02 or sng_co2 > 0.02:
9          return False
10
11     return True
12
13
14 def gw():
15     if not has_passed_constraints():
16         return numpy.nan
17     ipcc = ("IPCC 2013 no LT", "climate change", "GWP 100a")
18     return e2d.project.lca.scores.get(ipcc)
19
20
21 def lcop():
22     if not has_passed_constraints():
23         return numpy.nan
24     return e2d.project.lcc.results.lcop
25
26
27 def eff_storage():
28     if not has_passed_constraints():
29         return numpy.nan
30
31     sng = e2d.project.simulation.streams["N-SYNGAS"]
32     sng_ch4 = sng.composition["CH4"].output.mole_frac()
33     sng_h2 = sng.composition["H2"].output.mole_frac()
34     sng_co = sng.composition["CO"].output.mole_frac()
35
36     sng_lhv = sng_ch4 * 35.8 + sng_h2 * 10.8 + sng_co * 12.6  # MJ/cum
37     sng_volume_flow, _ = sng.output.total_volume_flow()
38
39     h2_in = e2d.project.simulation.streams["H2"]
40     h2_in_mass_flow, _ = h2_in.output.total_mass_flow()
41     h2_rec = e2d.project.simulation.streams["H2-REC"]
42     h2_rec_mass_flow, _ = h2_rec.output.total_mass_flow()
43     h2_mass_flow = h2_in_mass_flow - h2_rec_mass_flow
44
45     wind_power = 49 * h2_mass_flow
46
47     surplus_power, _ = e2d.project.simulation.utilities["ELECTRICITY"].total_value
48
49     eff = (sng_lhv * sng_volume_flow / 3600 * 1000) / (49 * wind_power + surplus_power)
50
51     return eff
52
```

Figure 50. Optimization objectives definition in eco2des.

A function to evaluate if the problem constraints are satisfied or nor is defined from line 1 to line 11. This function uses the methods from e2dsimulation module to get the composition of the SNG and check in line 8 if the constraints defined in Table 11 are met. This function is used in each objective function to insert the death penalty. Hence, when the constraints are not satisfied, the objectives functions return not a number using the capabilities of NumPy library (Harris et al. 2020). This is shown in lines 15 and 16, lines 22 and 23, and lines 28 and 29 in Figure 50.

Then, the three objective functions are defined:

- Global warming potential impact (GWP) is read from the `scores` attribute of the `lca` object of the project. This attribute is a mapping object that stores the LCIA results for each impact assessment category introduced when the LCA model is built. Therefore, the impact assessment category tuple is used as key to get the score value (lines 17 and 18).
- LCOP is read from the `results` object of the `lcc` object of the project as it is shown in line 24 of Figure 50.
- $\eta_{storage}$ is computed dividing the power of the SNG based on its LHV by the electricity power needed to produce the H_2 minus the electricity surplus produced in the plant. Therefore, from line 31 to line 34 the composition of the SNG is read from the simulation. Then, these values are used to compute the LHV of the SNG in line 36. In the next line, the volume flow of SNG produced by the plant is retrieved from the simulation. Then, from line 39 to line 43 the total mass flow of hydrogen that is fed into the plant from the electrolysis is calculated. This value is used in line 45 to compute the power demanded from the wind farm to produce the hydrogen. In line 47, the electricity that the plant is producing or demanding is read from the utilities of the simulation. Finally, in line 49 the storage efficiency is computed.

The next step is to define the decision variables as functions that change some inputs of the process simulation and return the value of the decision variable (Figure 51).

```
1  def h2_co2_ratio(var: float) -> float:
2      h2_in = e2d.project.simulation.streams["H2"]
3      h2_in_mole_flow, _ = h2_in.output.total_flow(basis="MOLE")
4      co2_in = e2d.project.simulation.streams["CO2"]
5      co2_in_flow = h2_in_mole_flow / var
6      co2_in.input.total_flow(value=co2_in_flow, basis="MOLE", unit="kmol/hr")
7      return var
8
9
10 def reactor_temp(var: float) -> float:
11     rplug = e2d.project.simulation.blocks["REACTOR1"]
12     rplug.input.temperature(value=var, unit="C")
13     return var
14
15
16 def reactor_length(var: float) -> float:
17     rplug = e2d.project.simulation.blocks["REACTOR1"]
18     rplug.input.length(value=var, unit="m")
19     return var
20
21
22 def reactor_ld_ratio(var: float) -> float:
23     rplug = e2d.project.simulation.blocks["REACTOR1"]
24     length, _ = rplug.output.length()
25     rplug.input.diameter(value=length / var, unit="m")
26     return var
27
28
29 def working_fluid(var: int) -> int:
30
31     working_fluid = e2d.project.simulation.streams["WFLUID-1"]
32     h2o = working_fluid.composition["H2O"]
33     cyclopentane = working_fluid.composition["CYCLOPEN"]
34
35     if var == 0:
36         h2o.input.flow(value=1, basis="MOLE-FRAC")
37         cyclopentane.input.flow(value=0, basis="MOLE-FRAC")
38     else:
39         h2o.input.flow(value=0, basis="MOLE-FRAC")
40         cyclopentane.input.flow(value=1, basis="MOLE-FRAC")
41
42     return var
43
```

Figure 51. Optimization decision variables definition in eco2des.

There are five decision variables in the optimization problem:

- First is hydrogen to carbon dioxide ratio. It is defined from line 1 to 7. To define it in the simulation, the H2 stream (Figure 39) total mole flow is read in lines 2 and 3. Then, the CO2 stream (Figure 39) object is retrieved in line 4. In line 5, using the ratio value the total mole flow of carbon dioxide is calculated and it is modified in the simulation in line 6, in order to modify the simulation values the methods of the `input` object of a simulation entity are used.

- The function to vary the temperature of the reactor (REACTOR 1 in Figure 39) is defined from lines 10 to 13.
- The reactor length is modified with the function defined in lines 16 to 19.
- Then the reactor length to diameter ratio which is set in function from lines 22 to 26. Here the length defined in the previous function is read in line 24 and the diameter of the reactor is modified accordingly in line 25.
- Finally, the working fluid topological variable is modified in the function from line 29 to 42. This decision variable is an integer. When it has a value of 0, the composition of the working fluid stream (WFLUID-1 in Figure 39) is modified to be water. On the other hand, if the value is 1 it is set to be cyclopentane.

To conclude, Figure 52 shows how to pick an algorithm defining the number of generations from e2doptimization module in line 1 and build the optimization problem from lines 3 to 13, including the decision variables as a tuple, their bounds as a tuple of two lists that contains the lower and the upper limits values (notice that the first value of each list must be the lower and the upper bound of the first element in the decision variables tuple. Finally, a tuple with the objective functions is passed as argument. `e2d.project.optimization.problem` is a factory method that builds an `OptimizationProblem` object that pygmo is able to handle. Then, a random initial population of 190 individuals is instantiated in line 15 and it is evolved with the selected optimization algorithm in line 17.

```
algorithm = e2d.optimization.moead(gen=20)

problem = e2d.project.optimization.problem(
    variables=(
        h2_co2_ratio,
        reactor_temp,
        reactor_length,
        reactor_ld_ratio,
        working_fluid,
    ),
    bounds=([4, 250, 1, 1, 0], [5, 400, 20, 10, 1]),
    objectives=(gw, lcop, eff_storage),
)

initial_population = e2d.project.optimization.population(problem, 190)

evolved_population = algorithm.evolve(initial_population)

```

Figure 52. Multi-objective problem definition and resolution in eco2des.

7.2.6. Life cycle interpretation

7.2.6.1. Evaluation

Multi-objective optimization problem 1

The optimization results of MOOP1 are presented in Figure 53. The problem was solved using MOEA/D algorithm with the Tchebycheff decomposition method (Ma et al. 2018) and the following parameters: population size, 190; evolutions, 20; size of the weight's neighborhood, 20; crossover parameter, 1; parameter for the differential evolution operator, 0.5; distribution index used by the polynomial mutation, 20.

The decision variables and objectives of the Pareto front of MOOP1 may be consulted in the APPENDIX A: Decision and objective vectors of the MOOPs.

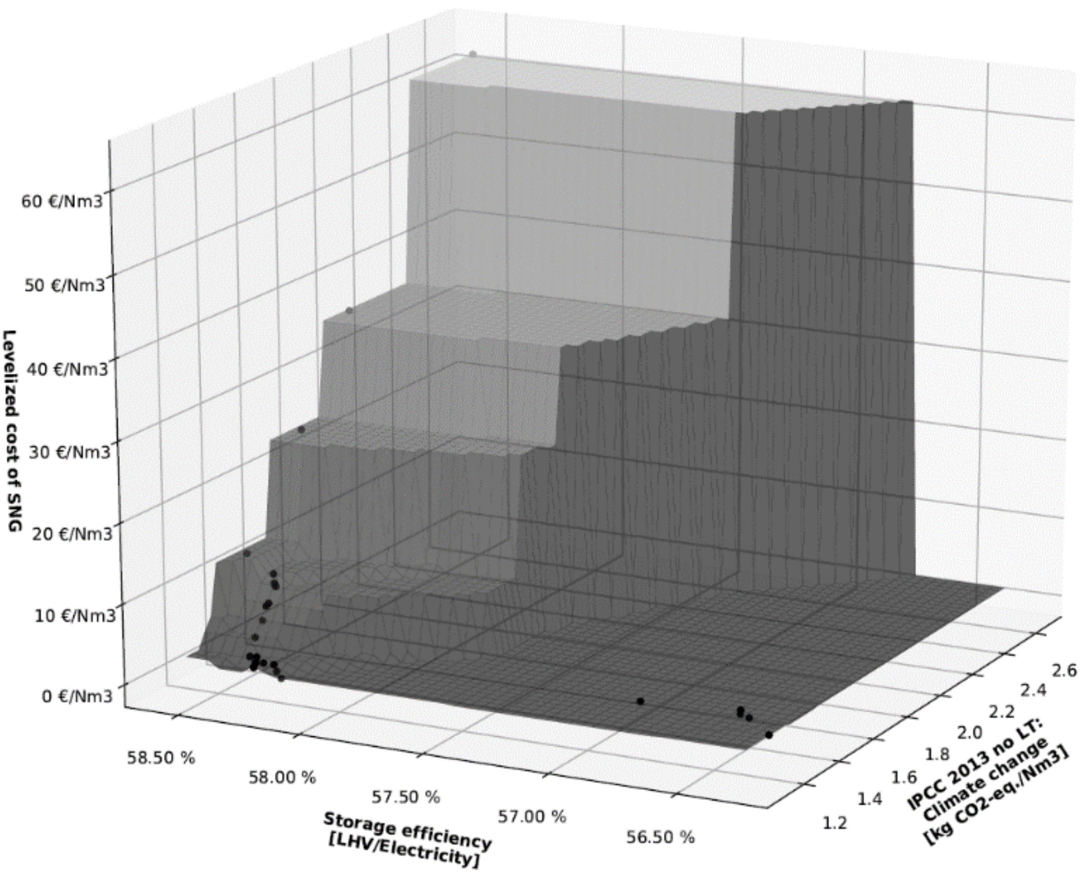

Figure 53. Optimization results for MOOP1: Pareto front

As the Pareto front shows, LCOP and GWP are non-conflicting objectives. Hence, when LCOP is minimized, GWP is as well. On the other hand, storage efficiency is conflicting with both. Consequently, MOOP2 was conducted.

Multi-objective optimization problem 2

The optimization results of MOOP2 are presented in Figure 54. The problem was solved using NSGA-II algorithm with the following parameters: population size, 200; evolutions, 20, crossover probability, 0.95; distribution index for crossover, 10; mutation probability, 0.01; distribution index for mutation, 50.

Also, the decision variables and objectives of the Pareto front of MOOP2 may be consulted in the APPENDIX A: Decision and objective vectors of the MOOPs.

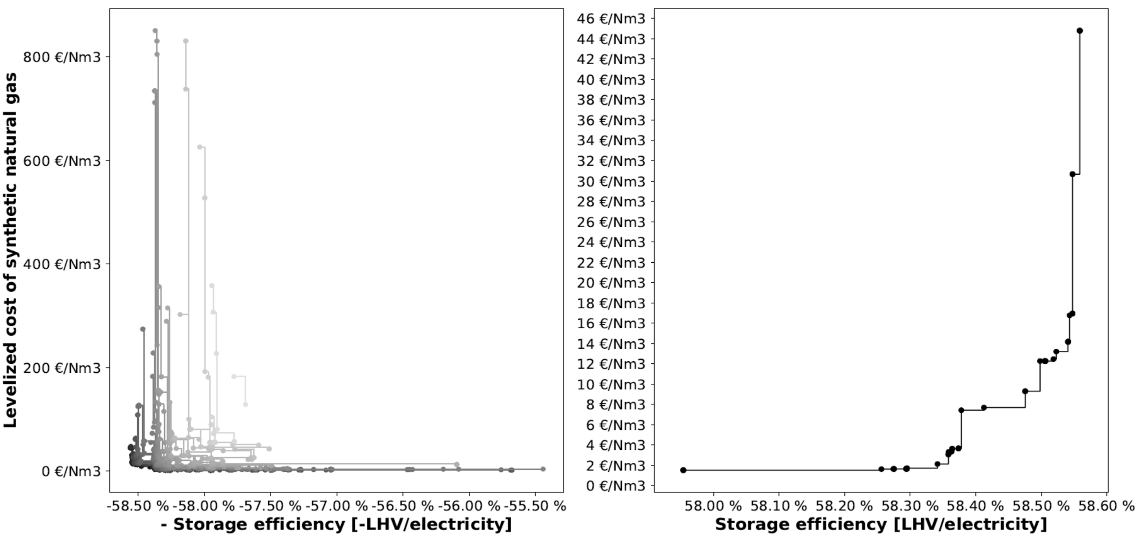

Figure 54. Optimization results for MOOP2: Population evolution (left) and Pareto front (right).

7.2.6.2. Discussion

The carbon dioxide methanation for wind energy storage in the natural gas grid problem with the decision variables detailed in Table 11 has non-conflicting environmental and economic performance. Regarding H_2/CO_2 ratio, all the scenarios computed in both Pareto fronts vary from the stoichiometric relation of 4 to 4.5. Optimal reactor temperature varies from 285 ^{o}C to 400 ^{o}C, the lower bound is achieved when the reactor is large enough to have a reaction dominated by the thermodynamic equilibrium instead by the kinetics of the reaction. Therefore, the maximum storage efficiency is achieved in scenarios with a H_2/CO_2 ratio near to the stoichiometric relation, a temperature of 285 ^{o}C, a reactor length of 16.83 m and a length to diameter ratio of 7.92. Furthermore, in these scenarios cyclopentane is used as working fluid, because, at lower temperatures, it gets a Rankine cycle more efficient than water increasing the electricity surplus in the plant and, therefore, plant storage efficiency. However, having a larger reactor and using cyclopentane as working fluid instead of water imply an increasing in the CAPEX and OPEX of the process, as well as an increasing in the global warming indicator because despite of producing more electricity using cyclopentane which decreases the LCI contribution of 'electricity production, wind, >3MW turbine, onshore, ES' activity; the contribution of technosphere activities related to the working fluid use is higher and more relevant in the impact assessment.

Anyways, the increasing performance in terms of storage efficiency is minuscule. The best scenario in these terms only outperformed the best scenario in economic and environmental terms on a 1 %. While, it has a LCOP 24 times higher and a GWP almost 2 times higher. Consequently, following the results of the eco2des evaluation, an optimization based on non-conflicting environmental and economic performance is recommended for this process design. This way, a LCOP of 1.48 €/Nm^3, GWP impact of 1.09 kg CO_2-eq./Nm^3 and a storage efficiency of 57.95 % are achieved with a H_2/CO_2 ratio of 4.44, a reactor temperature of 396 ^{o}C, a reactor length of 2.64 m, a reactor length to diameter ratio of 5.72 and using water as working fluid. Finally, in this configuration, a hydrogen recovery system is required, but carbon dioxide conversion is 98.63 % which allows SNG injection to the grid without recovering it.

7.2.6.3. Conclusions

The capabilities of eco2des, a novel Python framework for sustainability-based optimization of industrial processes, and how to carry out an eco-design with this Python tool have been presented in this case study. The tool encapsulates a novel framework which integrates process simulation, LCA, LCC and multi-objective optimization algorithms. The capabilities of the tool and its usage have been proved with its application in a case study under research, the carbon dioxide methanation for wind energy storage in the natural gas grid. The case study results clearly indicate the way for the detailed engineering in the development of this process, showing the best operational variables and process topology decisions to minimize costs and environmental impacts without compromising the storage efficiency of the system. This way, eco2des has demonstrate its viability as powerful decision support system (DSS) for the process engineering. Its application in early research phases allows for the optimization of resource allocation in projects with real sustainable potential. Furthermore, its application in processes under development may accelerate their time-to-value.

7.3. Biofuels production

7.3.1. Background

The depletion of fossil fuels and global warming are increasing the demand of clean and renewable fuel sources. By 2030, the European Union (EU) aims to have 14% of the transport fuel of every EU country coming from renewable sources, as stated in the recast of the Renewable Energy Directive (REDII) (*Directive (EU) 2018/2001 of the European Parliament and of the Council of 11 December 2018 on the Promotion of the Use of Energy from Renewable Sources (Recast) (Text with EEA Relevance.)* 2018). Within this 14% transport goal, there is a dedicated target for advanced biofuels produced from feedstock such as algae, biowaste, straw or manure among others. The contribution of advanced biofuels as a share of final consumption of energy in the transport sector shall be at least 1 % in 2025 and at least 3,5 % in 2030. Furthermore, there is a special concern about jet fuels. Direct emissions from civil aviation account for about 3% of total greenhouse gas emissions in the EU (*Regulation (EU) 2017/2392 of the European Parliament and of the Council of 13 December 2017 Amending Directive 2003/87/EC to Continue Current Limitations of Scope for Aviation Activities and to Prepare to Implement a Global Market-Based Measure from 2021* 2017). Biofuels can help lowering the EU's carbon footprint by providing a renewable alternative to jet fuel in airliners. They emit less CO_2, contain no sulfur compounds, and are generally more efficient due to their higher energy density (European Commission 2013). EU RED II outlines different variant scenarios for sustainable aviation fuels used in EU, accounting up to 5.25 % of EU air fuel demand.

As a promising route for the conversion of biomass into jet fuels, the integration of gasification with Fischer-Tropsch (FT) synthesis is one of the most increasingly studied pathways (Santos and Alencar 2020; Sims et al. 2010) thanks to some attractive advantages: no need for CO_2 capture and storage due to its biogenic nature, similar characteristics to petroleum derived fuels, near zero sulfur content, no need for blending with petroleum-based fuels (as e.g. biodiesel from oil crops) and compatibility with available infrastructure for transportation, storage and vehicle engines. FT synthesis has been industrially proven technically feasible for a variety of liquid fuels such as diesel, gasoline and kerosene from syngas. Nowadays, there are several plants around the world that produce FT liquids (Lappas and Heracleous 2016) but the commercial production of FT liquids from biomass is still some way off.

The biggest bottleneck for the market uptake of FT biofuels is their high capital costs which produces a lack of competitiveness in today's energy markets (Brown and Wright 2014). Public support to biofuels may overcome this in the short-term future, providing the market with a driver to ensure market penetration. For such approach, the development of sustainable biomass to liquid, BTL, processes lead to a favorable performance from a combined economic and environmental point of view.

In fact, the technical, economic and environmental aspects of BTL processes have been extensively studied. Tijmensen et al. reported that the overall thermal efficiency of a BTL process on a lower heating value (LHV) basis was 33–40% for gasification systems at atmospheric pressure and 42–50% for pressurized gasification systems (Tijmensen et al. 2002). The production costs of FT liquid fuels in a BTL process were found to be from 2 to 4 times higher than those of petroleum-derived fuels (Hamelinck et al. 2004; Rafati et al. 2017). FT synthesis requires syngas with a proper H_2/CO ratio regarding the final desired product. The optimal value depends on the catalyst and temperature used in the reactor: 2.15 for low-temperature cobalt, 1.65 for low-temperature iron, and 1.0 for high-temperature iron-based processes (Dry 2002). Leibbrandt et al. reported that a gasification process operated with a moderate steam-to-biomass ratio followed by a downstream shift reactor would achieve higher thermal efficiency than the use of only a gasifier operated at a high steam-to-biomass ratio to produce syngas with a proper H_2/CO ratio (Leibbrandt et al. 2013). Iribarren et al. concluded that FT fuels from biomass have a global warming potential a 70% lower than fossil fuels in a well-to-wheels assessment (Iribarren, Susmozas, and Dufour 2013), making them definable as renewable fuels for transport according to the criteria of the renewable energy directive in Europe (*Directive (EU) 2018/2001 of the European Parliament and of the Council of 11 December 2018 on the Promotion of the Use of Energy from Renewable Sources (Recast) (Text with EEA Relevance.)* 2018).

In order to accelerate the adoption of BTL technologies delineated above, the eco-design framework for industrial processes, as expounded upon in Section 5, is employed in the present case study. However, this study refrains from delving into the implementation specifics within the eco2des tool, as the prior case study has sufficiently addressed this aspect. Rather, the emphasis is placed on the application of the eco-design methodology to a more complex project, with the aim of showcasing the significance of this approach in offering valuable insights throughout the sustainable development of emerging technologies.

7.3.2. Goal and scope definition

The goal of this study is to environmentally and economically optimize the FT refinery for the coproduction of synthetic biofuels and electricity, using a life cycle perspective. The evaluated foreground system is shown in Figure 55, which covers the supply of biomass and raw materials and energy input into the process and the production of fuels. Previous works show that, in order to make the process economically feasible, the plant should treat 2,000 ton/day of dried biomass (Hamelinck et al. 2004; Leibbrandt et al. 2013; Rafati et al. 2017). In line with these works, the hypothetical plant of this study was selected accordingly and equal to that value in a first iteration. However, during the life cycle interpretation phase while establishing the reference case scenario this value is augmented to 2,800 ton/day. This decision is expanded in the following sections, supported by a scale-up study using the eco2des tool.

For the background system in the LCA analysis, the ecoinvent 3.6 version (Wernet et al. 2016) with the Cut-Off system model is used to model the value chain. While for the LCC model, this study uses present worth method to compute capital expenditures (CAPEX) and operational expenditure (OPEX) over the whole life cycle of the biorefinery not considering externalities. The cost of the principal equipment is taken from the literature and accordingly scaled to the product system's scale.

A cradle-to-gate approach was chosen for the system boundaries. Since the optimization was made over process design parameters, this approach was considered sufficient to ensure the production of biofuels while minimizing the environmental and economic impacts in a cradle-to-wheel analysis. Consequently, the emissions and costs upon combustion of the fuel were chosen to fall out of the scope of the assessment, since these fuels are not compared with conventional fuels or other biofuels, but with other process alternatives during the optimization.

The functional unit (FU) of the system is 1 kWh of fuels (hydrogen, gasoline, kerosene and diesel) using their lower heating value, produced as detailed during the process simulation description. According to that FU, two environmental impact categories are evaluated: global warming (GW) and fossil depletion (FD). Furthermore, net present value (NPV) is implemented as a measure of economic performance.

7.3.2.1. Problem statement

Given:

- A process superstructure of potential topological and operational alternatives of the synthetic fuels production from biomass, based on its simulation defined by thermodynamics and kinetics relationships, and mass and energy balances.
- A lifetime, the price of the final products, the cost of the equipment, raw materials and utilities.
- The environmental burdens of the upstream activities of the value chain.

The problem then consists of optimizing the production process using its operational variables, minimizing the environmental impacts and costs, and maximizing the kerosene production over the entire lifetime.

7.3.3. Predictive life cycle inventory analysis

7.3.3.1. Process simulation

The refinery configuration in this study only includes commercially available technologies that are thus ready for their deployment in the proposed biomass gasification with Fischer-Tropsch processing. Figure 55 shows a general scheme with the main steps for producing FT fuels and power, where ASU is the air separation unit, WGS is the water gas shift reactor, AGR is the acid gas removal part, FT is the Fischer-Tropsch synthesis, PSA is the pressure swing adsorption unit, ATR is the auto-thermal reforming reactor and HC is the hydrocracking unit.

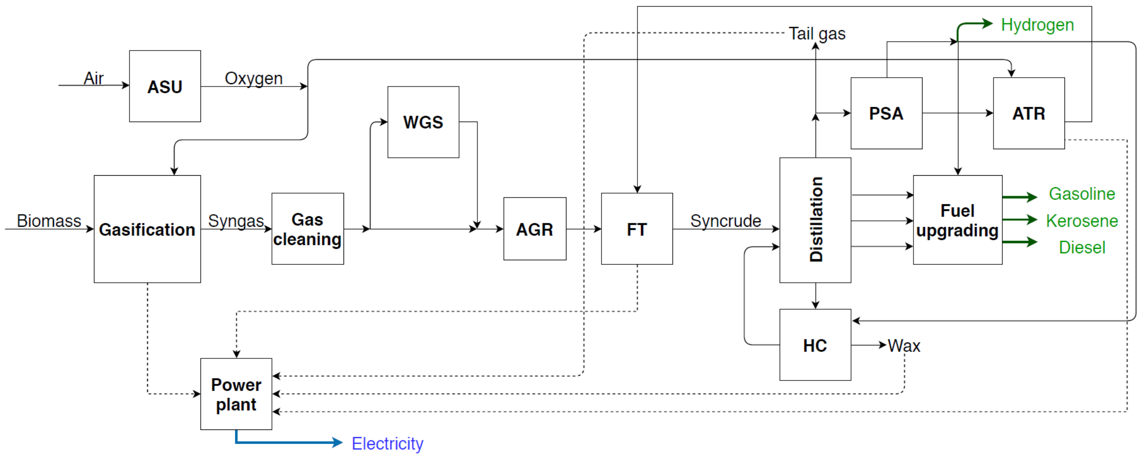

Figure 55. Bio-refinery flowchart diagram. The dashed line represents heat flows.

Syngas from gasification can be produced from several feedstock: biomass, coal, petroleum coke or municipal solid waste. This study focuses on biomass (corn cob in this case), but the model is ready for any carbon-based solid feedstock if defined through its ultimate and proximate analysis. The syngas requires additional processing to remove possible contaminants and impurities such as particulates, sulfur and nitrogen compounds. Furthermore, the syngas for a FT process might require adjusting the H_2/CO ratio and to remove CO_2 content. The cleaned and conditioned syngas is then converted to hydrocarbons in a FT synthesis reactor. The products of FT synthesis are then separated and upgraded into different liquid fuels using similar unit operations to those that can be found in a petroleum refinery (Steynberg and Nel 2004). The tail gas from distillation is injected into a PSA unit in which hydrogen is recovered for fuel upgrading processes, fitting the H2/CO ratio of recirculated syngas and as final product. Then an ATR converts light hydrocarbons into syngas which is recirculated. Also, waxes from distillation are cracked for recirculation into the distillation train. The integrated process configuration was modelled in Aspen Plus using the Soave-Redlich-Kwong, SRK, equation of state, except pure water streams which used the NBS/NRC steam tables.

Gasification

Figure 56 shows the Aspen Plus flow diagram for the gasification step. First, the biomass is crushed and fed into an air dryer to remove the excess of water. Biomass crushing was not integrated into the simulation model, but its electricity consumption was modelled as 0.02 kWe/kWt (Van der Drift et al. 2004) for inventory purposes. In the drying step, the air is introduced at 140 ºC and its amount is computed with a design specification to obtain a biomass with a 5% of moisture after drying. In the gasification, high purity oxygen was assumed to be generated in an air separation unit, ASU, not implemented into the simulation but the consumption of utilities (electricity, cooling water and heat as steam) are modelled with correlations from Clausen, Houbak, and Elmegaard (2010). Oxygen, woody biomass and steam are fed to a downward entrained-flow gasifier. The system was modelled as a 0-D system considering two stages: decomposition and gasification. The model strategy of Scott and Adams II (2018) was used. The overall approach consisted of a first theoretical decomposition of biomass into a mixture of solid carbon, solid sulfur, water, hydrogen gas and chlorine gas. Then, the gasifier output is estimated by assuming chemical equilibrium at 25 bar using the gasification temperature and the amount of steam, decision variables of the optimization problem, while calculating the oxygen flow in order to maintain the temperature in the gasifier.

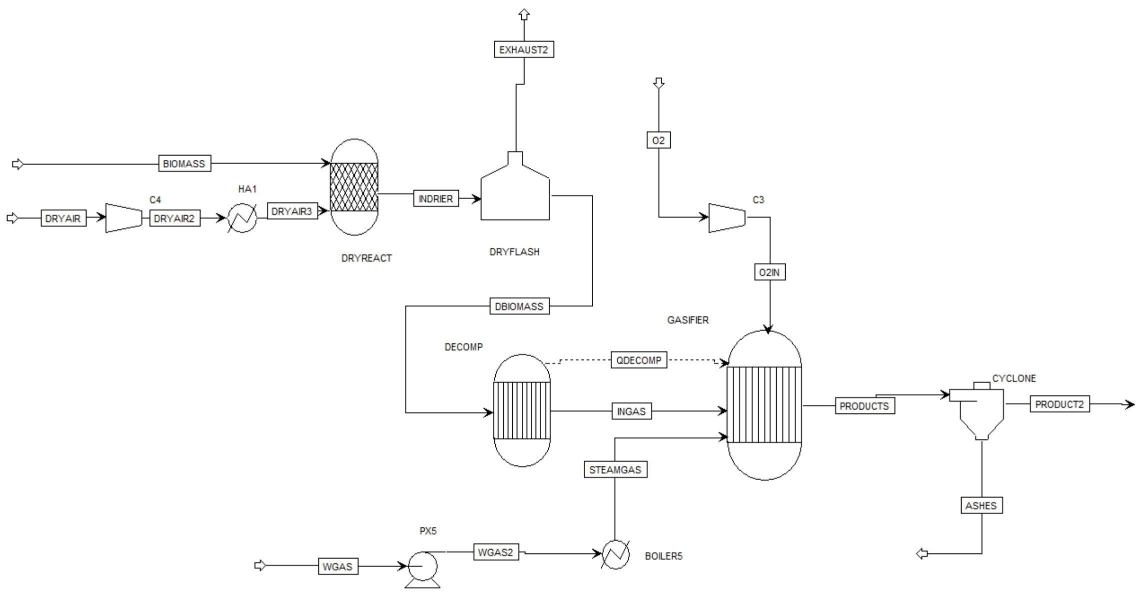

Figure 56. Gasification flowsheet

Gas cleaning, water gas shift and acid gas removal

Figure 57 shows the Aspen Plus flow diagram for the gas conditioning step. The syngas may contain different types of contaminants such as particulates, tar compounds, alkali compounds, H_2S, COS, HCN, NH_3 and HCl in various quantities depending on the source of biomass and operating conditions of the gasifier. These contaminants would create important corrosion problems, as well as catalysts deactivation in downstream processes, such as poisoning of FT catalysts by sulfur (Woolcock and Brown 2013; Karn et al. 1963).

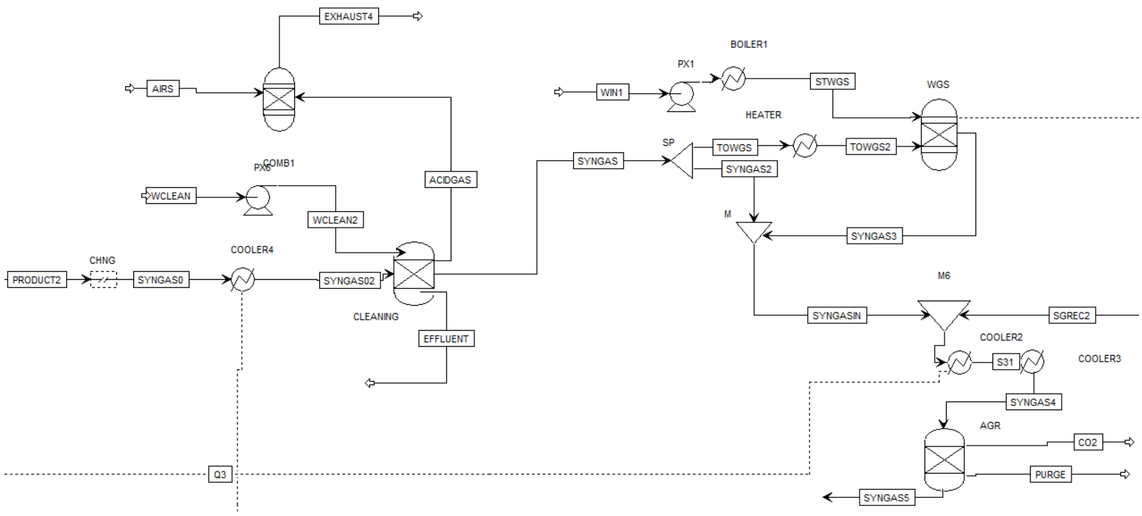

Figure 57. Gas cooling, cleaning, WGS and AGR flowsheet

Thus, several cleaning steps are included. Cold syngas cleaning, assumed in this study, is an industrially proven technology. After the removal of particulates in a cyclone, syngas is cooled down to a temperature of 88 ºC, using this heat to produce steam for heat recovery and power production. Then, water scrubbers remove several contaminants including particulate matter, nitrogen compounds and tars. Finally, if syngas sulfur compounds content is higher than 50 ppm, they must be removed. For biomass, a ZnO guard bed is a proper technology for their removal (Chiche et al. 2013). Since gas cleaning was not considered within the optimization scope of this study, these steps were modelled as black box separation units in the Aspen Plus simulation, where a single reaction yield was assumed. Also, reactivation of the guard bed is modelled with the combustion of the sulfur compounds with an RGibbs reactor. The waste sour water from scrubbers is neutralized, using a Python script in order to estimate the amount of neutralizing agent needed.

The H_2/CO ratio in the syngas is a design parameter in this model, which affects the performance of the FT synthesis. This ratio can be adjusted in a WGS unit in which H_2O reacts with CO to produce H_2 according to the following reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H^o_{298} = -41 \ {}^{kJ}/_{mol}$$

A sour water-gas shift process with an iron-chromium-magnesium catalyst is used in this study. It was modelled using an adiabatic Gibbs reactor under a restricted equilibrium option. The reactor is placed in a split stream and the split ratio is adjusted through a design specification in Aspen Plus in order to obtain the targeted H_2/CO ratio.

The syngas from the gasifier also contains a large amount of CO_2 which is further increased during the WGS reaction. The presence of CO2 in the syngas would lower the yield of liquid hydrocarbons in the FT synthesis, especially when a cobalt-based catalyst is chosen (Gnanamani et al. 2011). So, a Rectisol process is used to remove CO_2 and other acid gases. It is selected over other processes such as MDEA because it has a lower energy consumption (Cormos, 2011). The Rectisol process is assumed to remove up to 97% of CO_2 (Leibbrandt et al., 2013). As well as in the other cleaning steps, a black box separator is used in Aspen Plus. Heating and cooling duties (0.0622 and 0.1553 kWh/kg-CO_2), and methanol make-up (0.3 wt. %) were introduced in the model from correlations taken from the literature (Cormos 2011).

Fischer-Tropsch synthesis

The FT synthesis may operate in two main modes: low-temperature (LTFT) from 200 to 250 ºC to mainly produce longer chain fuels, i.e., diesel, and high-temperature (HTFT) from 300 to 350 ºC to produce shorter chains, targeting mainly gasoline. In this study, a LTFT mode in a slurry bubble column FT reactor was chosen to focus on kerosene production.

The kinetics applied are taken from (Rafati et al. 2017). It is reported in term of the rate of CO in moles converted to products per mass unit of the catalyst. The product distribution of FT synthesis in this study assumes to follow the theoretical Anderson-Schulz-Flory (ASF) distribution based on the chain growth probability values (Visconti and Mascellaro 2013):

$$m_{C_n} = \alpha^{n-1}(1-\alpha)$$

$$\alpha = \left[b\left(\frac{(H_2/CO)_{in}}{(H_2/CO)_{ref}}\right)^{\beta} + c\left(\frac{GHSV}{GHSV_{ref}}\right)^{\gamma} + d\left(\frac{(Y_{inerts})_{in}}{(Y_{inerts})_{ref}}\right)^{\delta} + e\left(\frac{T}{T_{ref}}\right)^{\varepsilon} \right]^{-1}$$

Where α is the probability of the chain growth and m_{C_n} is the mole fraction of hydrocarbons with n carbon atoms. The α correlation considers the H_2/CO ratio (mol/mol), the gas space velocity over catalyst mass, GHSV, the amount of inert compounds, Y_{inerts}, and the reactor temperature, T (K). Reference values and constants b, c, d, e, β, ϒ, δ and ε were taken from Visconti and Mascellaro, 2013. For this analysis, it was assumed that alkanes are the only products of FT synthesis.

Kinetics and product distribution model were introduced through a calculator block in the Aspen Plus simulation. The model was built to calculate the syngas conversion efficiency for a given syngas composition, GHSV, the reactor temperature and the molar distribution of hydrocarbons up to C28.

Auto-thermal reforming and pressure swing adsorption

Figure 58 shows the Aspen Plus flowsheet for this section. The FT synthesis products are cooled down to separate the tail gas from liquid and waxes. Tail gas from first flash separation and from the distillation train contains a huge amount of hydrogen and light hydrocarbons. First, a pressure swing adsorption, PSA, unit is used for recovering the hydrogen operating at 40 °C and 28 bar. For the sake of simplicity, it was modelled as a black box recovering the 85% of the hydrogen with a high purity of 99.99% (Susmozas, Ana 2015), which is then recirculated to the upgrading processes: hydrocracking, hydrothermal treatment and isomerization. A design specification evaluates if the recovered hydrogen is enough to satisfy the demand, then a hydrogen make-up or production is computed considering the hydrogen production in the reforming of liquid fuels and the hydrogen needed to adjust the H_2/CO ratio of the recycled syngas. Second, the unreacted syngas, enriched in light hydrocarbons, is fed to a reformer to produce syngas which is recirculated into the FT synthesis. A purge is in any case needed to avoid accumulation of inert compounds such as CO_2. The syngas purged is used to produce steam with heat calculated in a Gibbs energy minimization (RGibbs) combustion reactor.

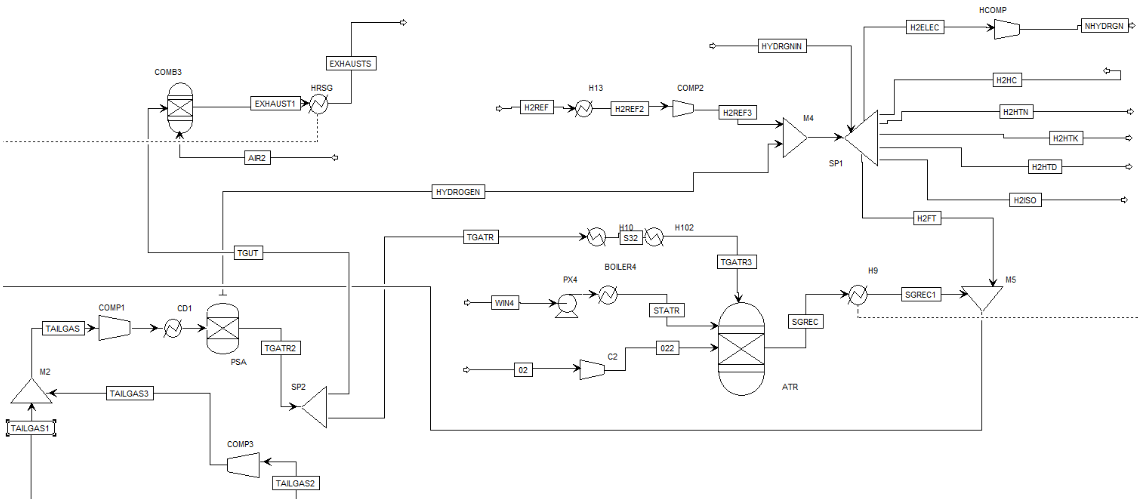

Figure 58. ATR, PSA and hydrogen distribution flowsheet in Aspen Plus

In this study, an autothermal reformer (ATR) was assumed in which the highly endothermic reforming reaction is provided by the partial oxidation of the light hydrocarbons. Also, along the WGS reaction, light hydrocarbons react with steam to produce additional H_2 and CO according to the following reaction:

$$C_nH_m + nH_2O \rightarrow nCO + \left(n + \frac{m}{2}\right) H_2$$

When CO_2 exits in the feed, dry-reforming reaction also takes place:

$$C_nH_m + nCO_2 \rightarrow \frac{m}{2} H_2 + 2nCO$$

The reforming reactor is typically operated at a temperature higher than 800 °C in the presence of a nickel-based catalyst (Mortensen and Dybkjær 2015). In Aspen Plus, a Gibbs reactor was used to model the ATR unit. The oxygen required is produced in the ASU and its amount was controlled using a design specification to have a 0 duty production at 900 ºC. Although the theoretical molar ratio of steam to carbon is 1:1, an excess of steam (1.1:1) was used to avoid coke formation (Aasberg-Petersen et al. 2003).

Synthetic fuels upgrading

Figure 59 shows the Aspen Plus flowsheet for the upgrading step. After FT synthesis, a distillation column is needed to separate the different hydrocarbons. This unit is analogue to the ones used in traditional refineries, so it is well-studied and well-optimized in the current state-of-the-art. Therefore, for the sake of simplicity, it was introduced as a separation block in the Aspen Plus simulation. The steam utility for the distillation column strippers were set to 1.2 wt. % (of syncrude) (Samborskaya et al. 2014). After distillation, different fuel cuts are obtained: naphtha, heavy naphtha, kerosene, diesel and wax. These need different upgrading processes before their introduction in the market. These processes are also analogue to the ones used in traditional refineries, so following the same approach as before they were not strictly simulated, but their consumption of utilities was calculated.

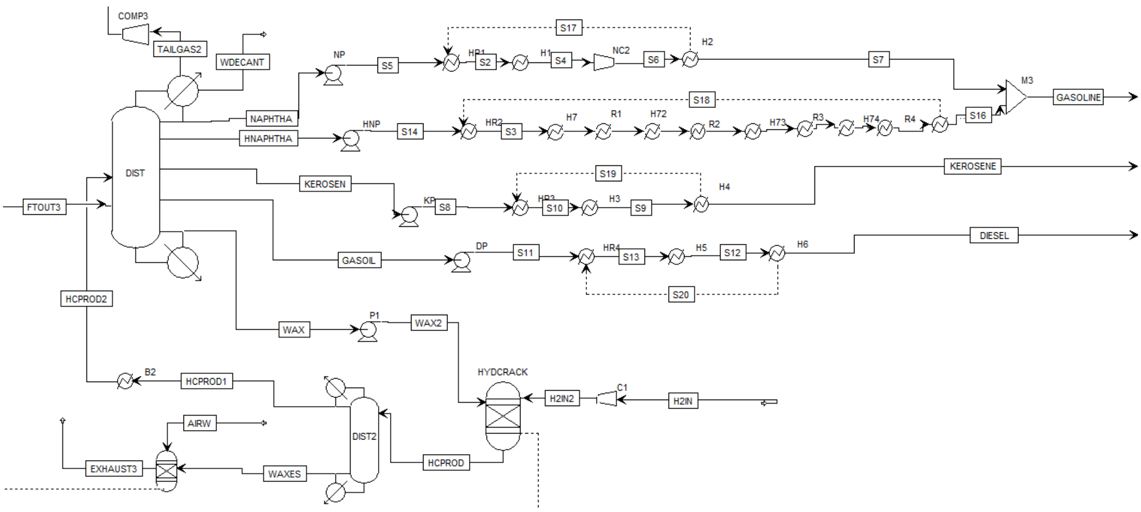

Figure 59. Synthetic fuels upgrading flowsheet

Hydrotreating is an important upgrading process in which desulfurization, denitrogenation, deoxidation, metals elimination and olefin saturation is simultaneously accomplished. It is an exothermic process which consumes hydrogen, and it is applied to each commercial cut: naphtha, diesel and kerosene. Cobalt-Molybdenum over alumina is the catalyst used, liquid hourly space velocity (LHSV), process conditions and hydrogen consumption were taken from literature (KLM Technology 2013) and represented in Table 12.

Table 12. Hydrotreating process conditions

Fuel	LHSV [h^{-1}]	Temperature [°C]	Pressure [bar]	H_2 consumption [m^3/bbl]
Naphtha	5	300	7	7
Kerosene	4	330	7	14
Diesel	2	340	10	28

A catalytic reforming is applied to heavy naphtha. This process produces high octane gasoline and hydrogen. A conventional configuration consists of 3 or 4 reactors in series and heaters before each reactor to reheat the stream into the reaction temperature range (450 – 550 ºC). In the Aspen Plus simulation, four reactors were assumed represented as heaters to model the endothermic character of the reaction and to compute the consumption of heat utility. The decrease of reactor temperature, pressure (10 bar), catalyst load (PtRe/Alumina) and hydrogen production (3 wt.% over heavy naphtha treated) were taken from literature (Shakoor 2011) and introduced in the model as correlations.

Light naphtha is fed to an isomerization unit. It is a catalytic exothermic process, which also uses PtRe/Alumina, in which straight chain paraffins are transformed into branched chains with the same carbon number but with higher octane numbers. LHSV (5 h^{-1}) and hydrogen consumption (1.1 wt. hydrogen to hydrocarbon ratio) were also taken from literature (Mencarelli, Pagot, and Duchêne 2020) and introduced in the model as correlations.

The wax cut is hydrocracked. Hydrocracking reactor operates at 100 bar and 360 C. The conversion and yields were taken from Hanaoka et al. (2015) and the hydrogen consumption is calculated in a calculator block to satisfy the atomic mass balance.

CHP unit

Figure 60 shows the Aspen Plus flowsheet for the heat integration scheme. Biorefinery excess heat is recovered in the process and generate steam for power production. There are two levels of steam used in this work: high pressure (HP) and medium pressure (MP). The demand for both types of steam is based on the biorefinery needs. The excess steam that is not consumed by the plant is sent through a steam turbine, which generate additional power for the plant.

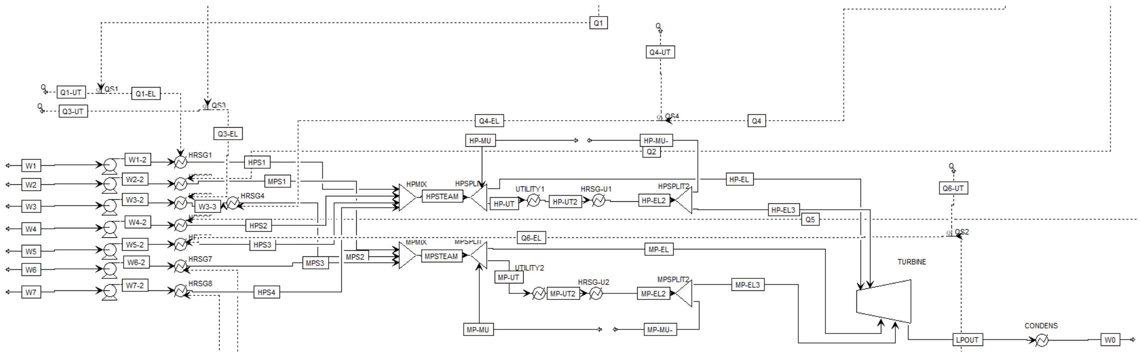

Figure 60. Heat recovery and power plant flowsheet

7.3.3.2. *Environmental inventory*

Tables 13 and 14 present the main inventory elements of the system. eco2des is used to link the process simulation to each element to create the predictive inventory of the BTL system.

Table 13. Biosphere inventory elements of the FT refinery (FU: 1 kWh of biofuels)

Elementary flow	Unit
Water, to air	cubic meter
Carbon dioxide, non-fossil, to non-urban air or from high stacks	Kilogram
Carbon monoxide, non-fossil, to non-urban air or from high stacks	Kilogram
Oxygen, to in air	Kilogram
Nitrogen, to in air	Kilogram
Nitrogen oxides, to non-urban air or from high stacks	Kilogram
Hydrochloric acid, to air	Kilogram
Chlorine, to non-urban air or from high stacks	Kilogram
Sulfur dioxide, to non-urban air or from high stacks	Kilogram
Sulfur trioxide, to non-urban air or from high stacks	Kilogram
Methanol, non-urban air or from high stacks	Kilogram
Water, cooling, unspecified natural origin, to in water	cubic meter

Therefore, the inventory data of the foreground system derive from the Aspen Plus process simulation. Data regarding the biomass feedstock production and other background processes were taken from the ecoinvent database (Wernet et al. 2016). Data presented in Table 14 shows the flows from the technosphere (i.e. manufactured goods and services) that are calculated per FU of the system, where $m_{biomass}$ is the biomass mass, moisture is the moisture content (w/w) of the biomass, and ash is the ash content (w/w) of the biomass. AspenCOM refers to the data taken from the link between eco2des and process simulation and the name in brackets refers to the variable from the process model: syngas is the volume of syngas produced in the gasification, energy from fuels is the kWh of biofuels produced (in LHV basis), neutralizer is the amount of sulfuric acid or sodium hydroxide needed for neutralizing the waste water from gas cleaning, oxygen is the mass of oxygen demanded by the biorefinery, softened water is the water mass demand for the power plant, water is the rest of water mass demand, waste water is the volume of waste water produced in the biorefinery, FT out is the mass of FT products which need to be distilled and upgraded, power is the electrical power of the power plant dimensioned for the biorefinery, electricity is the electricity surplus, modelled as avoiding the marginal production of combined cycles (assuming the plant is located in Spain) or demand in the biorefinery, and methanol is the methanol makeup for the Rectisol process.

For the technosphere inventory, activities for gasification materials (items 2, 3, 4, 5) were taken equal to the ecoinvent inventory for synthetic gas production, from wood, at a fluidized bed gasifier; adapted to the new FU of this study. Catalyst loads were computed following the equation:

$$catalyst = {}^{\dot{V}\ *\ \rho}/_{GHSV}$$

Where, $\dot{V}$ is the volumetric flow (taken from the Aspen Plus simulation) ρ is the catalyst density (assumed to be 1025 kg/m3 in all cases) and GHSV is the space velocity of the gas (values taken from literature (Kent 2007; Swanson et al. 2010; KLM Technology 2013), except for FT catalyst which is an input of the model). Hence in Table 14, ZnO is the zinc oxide guard bed, CoAl is the cobalt over alumina for the FT synthesis, CoMoAl is the cobalt and molybdenum over alumina for the biofuels hydrotreatment, NiMoAl is the nickel and molybdenum over alumina for the ATR reactor and the wax hydrocracking unit, FeCrMg is the iron, chromium and magnesium catalyst for the WGS reactor, and the PtReAl is the platinum and rhenium over alumina for the naphtha reforming and isomerization. Since the rhenium market or production are not integrated in ecoinvent version 3.6, this activity was modelled as market for selenium, as this activity has really close environmental impacts (Nuss and Eckelman 2014). Finally, catalysts are assumed to be recycled after their lifetime.

Table 14. Technosphere inventory data of the FT refinery (FU: 1 kWh of biofuels)

Inventory element	Amount*	Unit
market for wood chips, wet, measured as dry mass, Europe without Switzerland	$m_{biomass} * (1 - moisture)$	kg
market for wood ash mixture, pure, Europe without Switzerland	$- m_{biomass} * ash$	kg
market for dolomite, RER	$0{,}010157 * \frac{AspenCOM['syngas']}{AspenCOM['energy\ from\ fuels']}$	kg
market for zeolite, powder, GLO	$0{,}020803 * \frac{AspenCOM['syngas']}{AspenCOM['energy\ from\ fuels']}$	kg
market for waste zeolite, RoW	$- 0{,}020803 * \frac{AspenCOM['syngas']}{AspenCOM['energy\ from\ fuels']}$	kg
market for silica sand, GLO	$0{,}012598 * \frac{AspenCOM['syngas']}{AspenCOM['energy\ from\ fuels']}$	kg
market for sulfuric acid, RER or market for sodium hydroxide, without water, in 50% solution state, GLO	$AspenCOM['neutraliser'] * operating\ hours$	kg
market for zinc oxide, GLO	ZnO	kg
synthetic gas factory construction, CH	$\frac{m_{biomass} * 24 * operating\ hours * years}{35 * 7920 * 50}$	unit
air separation facility construction, RER	$\frac{AspenCOM['oxygen'] * years}{0{,}233 * 80000 * 20}$	unit
water production, completely softened, RER	$AspenCOM['water\ softened']$	kg
market for water, decarbonised, ES	$AspenCOM['water']$	kg
market for wastewater, from residence, RoW	$- AspenCOM['waste\ water']$	m^3
petroleum refinery construction, RER	$\frac{AspenCOM['FT\ out'] * years}{1e9 * 30}$	unit
gas power plant construction, 100MW electrical, RER	$\frac{AspenCOM['power'] * years}{100 * 30}$	unit

market for methanol, GLO	$AspenCOM['methanol'] * operating\ hours$	kg
market for cobalt, GLO	$(CoAl * 15\% + CoMoAl * 5\%) * {}^{1}/_{3}$	kg
market for molybdenum, GLO	$(CoMoAl * 10\% + NiMoAl * 10\%) * {}^{1}/_{3}$	kg
market for iron ore, crude ore, 46% Fe, GLO	$6\% * (FeCrMg * 74{,}2\%) * {}^{1}/_{3}$	kg
market for chromium oxide, flakes, GLO	$(FeCrMg * 10\%) * {}^{1}/_{3}$	kg
market for magnesium oxide, GLO	$(FeCrMg * 0{,}2\%) * {}^{1}/_{3}$	kg
market for nickel, 99.5%, GLO	$(NiMoAl * 5\%) * {}^{1}/_{3}$	kg
market for platinum, GLO	$(PtReAl * 0{,}3\%) * {}^{1}/_{10}$	kg
market for selenium, GLO	$(PtReAl * 0{,}3\%) * {}^{1}/_{10}$	kg
market for aluminium oxide, non-metallurgical, IAI Area, EU27 & EFTA	$(CoAl + CoMoAl + NiMoAl) * 75\% * {}^{1}/_{3} + PtReAl * 99.4\% * {}^{1}/_{10}$	kg
market for inert waste, for final disposal, RoW	$-(dolomite + silica\ sand)$	kg
electricity production, natural gas, combined cycle power plant, ES or market for electricity, medium voltage, ES	$-AspenCOM['electricity']$	kWh

*AspenCOM is the COM object used by eco2des to read data from Aspen Plus

7.3.3.3. Economic inventory

CAPEX estimation

CAPEX is calculated in the eco2des framework applying the factored estimation method (Towler and Sinnott 2013a) for the main equipment. The costs of principal components of the plant were computed using a scaling factor applying equation 6.

Reference values were taken from the literature (Holmgren 2015; Rafati et al. 2017; Susmozas, Ana 2015) as detailed in Table 15. Additional equipment costs such as pumps, compressors and heaters were estimated using the framework built-in correlations. For all of them, the capacity is linked to the simulation results to build the predictive economic inventory.

To address the average cost escalations in plant costs over the past years, the average annual Chemical Engineering Plant Cost Index (CEPCI) was used to convert from original-year monetary value to 2019 (Jenkins 2022).

Finally, catalyst preparation costs were assumed to double the cost of the raw materials. Raw material costs were introduced in eco2des from different online databases (Glacier Media Group 2020; The London Metal Exchange - an HKEX Company 2020; BASF SE 2020).

Table 15. Basic costs for major equipment

Equipment	Reference capacity	Reference cost, thousand EUR	Scale factor
Biomass storage, preparation and feed	64.6 tone/h (biomass)	2,940	0.77
Biomass air dryer	1.08 10^6 m^3/h (air)	84	0.8
CFB gasifier, gas cooling and gas cleaning	483 MW (biomass LHV)	151,840	0.5
ASU with O_2 and N_2 compressors	2202 tone / day (O_2)	60,371	0.5
Water gas shift reactor	2400 kmol/h (CO+H_2)	328,5	0.6
ATR Reactor	365 MMSCFD (tail gas)	21,827	0.67
PSA	155.24 tone/day (H_2)	7,319	0.7
Fischer-Tropsch slurry reactor	2420 MW (fuels)	246,310	0.75
Distillation recovery plant	3190 MW (fuels)	74,150	0.65
Wax hydrocracker	4.1 tone/h (wax)	6,789	0.55
Naphtha hydrotreater	0.93 tone/h (naphtha)	547	0.65
Kerosene hydrotreater	0.93 tone/h (naphtha)	547	0.62
Diesel hydrotreater	1.3 tone/h (diesel)	1,818	0.6
Isomerization unit	0.5443 tone/h (naphtha)	699	0.62
Heavy naphtha reformer	1.54221 tone/h (naphtha)	3,781	0.6
Rectisol	200,000 Nm^3/h (syngas)	21,024	0.63
HRSG	24 MWt	1,825	0.7
Steam cycle	275 MWe	48,691	0.7

MMSFCD: Million standard cubic feet per day; CFB: Circulating Fluidized Bed; ASU: Air Separation unit: ATR: Autothermal reformer; PSA: Pressure swing adsorption; HRSG: Heat Recovery Steam Generator

OPEX estimation

OPEX estimation is performed in the eco2des frameworks as detailed in Table 16, where ISBL is the inside battery limits costs and OSBL is the outside battery limits costs; both calculated in the CAPEX section through the factored estimation method. Finally, f() means that a function was introduced in the framework to model that cost.

Table 16. Operational expenditure calculations

Fixed costs	Maintenance	$5\% \cdot ISBL$
	Operating labor	$f()$
	Supervision	$25\% \cdot Operating\ labour$
	Plant overheads	$65\% \cdot (Operating\ labour + Supervision)$
	Capital charges	$f()$
	Environmental costs	$1\% \cdot (ISBL + OSBL)$
	Insurance	$1\% \cdot ISBL$
	License fees and royalties	$2.5\% \cdot Sales$
Variable costs	Raw materials	$f()$
	Utilities	$f()$
	Operating materials	$10\% * Maintenance$

Labor cost was estimated from the number of the job positions needed in the plant, considering that every position means 4.8 full time employees. On the one hand, positions for gasification, FT and refinery processes, and power plant were estimated as 1, 3 and 3, respectively, following literature estimates (Towler and Sinnott 2013b, 8). On the other hand, a correlation was built to estimate the positions needed in the solid handling plant. It uses the biomass mass flow, the biomass density, the volume of the machinery used to transport the biomass from the storage facilities to the gasification silo and the frequency of loading and discharging periods. Hence:

$$positions = \frac{biomass\ flow\ [\frac{m^3}{h}]}{frequency\ [h^{-1}] \cdot machinery\ volume\ [m^3]} \quad (14)$$

Capital charges depend on depreciation and loan payments which will be further detailed in the following section. The principal raw materials and utilities are biomass, methanol, sulphuric acid, sodium hydroxide, water, refrigeration water, softened water and electricity whose amounts are taken from the Aspen Plus simulation results and their prices are detailed in Table 17. Biomass cost in Spain was taken from official reports on prices and availability (IDAE 2019) and multiplied by a factor of 1.2 to account for the logistic costs.

Table 17. Raw materials and utilities prices.

Raw material / utility	Cost, €
Biomass, 1 kWh (LHV)	$1.2 \cdot 0.012$
Methanol, 1 kg	0.315
Sulphuric acid, 1 kg	0.034
Sodium hydroxide, 1 kg	0.545
Water, 1 tonne	0.48
Refrigeration water, 1 tonne	0.027
Softened water, 1 tonne	1.29
Electricity, 1 kWh	0.09

7.3.4. Life cycle impact assessment

7.3.4.1. Environmental impact assessment

Once the predictive life cycle inventory of the biorefinery was implemented into eco2des, two environmental impact categories were evaluated: global warming (GW) and fossil depletion (FD). GW was computed using the global warming potentials of the IPCC 2013 method (Stocker et al. 2013) without long term emissions and FD was calculated using ReCiPe Midpoint (H) v1.13 method (Huijbregts et al. 2016).

7.3.4.2. Economic impact assessment

Following the recommendations exposed in the petroleum and natural gas industries – Life cycle costing ISO series (ISO 2021), the nominal interest rate was set to 5% in this study. On the other hand, for assessing the NPV of the project sale prices need to be defined. For this study, Spanish market prices without taxes in 2020 were used as shown in Table 18.

Table 18. Sale prices for biorefinery products

Product	Market Price	Market Price per GJ
Gasoline	0.608 € / L	19.0 €
Kerosene	0.624 € / L	17.7 €
Diesel	0.640 € / L	17.8 €
Hydrogen	2.5 € / kg	20.8 €
Electricity	57 € / MWh	15.8 €

Finally, the model assumed a financial scheme of 40 % own resources and 60 % borrowed resources, with a loan with a 4 % of interest rate and ten years' period. A linear depreciation model with a value of 7 % per year was also included. The interannual cost variance assumed per cost element are shown in Table 19.

Table 19. Costs and benefits variance

Costs and benefits	Annual variance
Sale prices	+ 1.5 %
Maintenance cost	+ 2.5 %
Salaries	+ 1.5 %
Raw materials cost	+1.5 %
Utilities cost	+ 2 %

7.3.5. Multi-objective optimization

A first optimization problem with two objectives has been proposed to minimize the global warming impact and maximize the net present value. In a second optimization problem, the amount of kerosene was added as a third function to be optimized, since the objective is to maximize the application of the technology for aviation fuels. Both multi-objective optimization problems (MOOP) share five decision variables which are detailed in Table 20 and whose bounds were chosen by preliminary sensitivity analysis. Furthermore, these analyses show that GW and FD behave similarly in the optimization space, therefore, GW was selected as environmental objective.

Table 20. MOOPs formulation

Objective functions		
MOOP1	$Min(GW, -NPV)$	
MOOP2	$Min(GW, -NPV, -Kerosene_{production})$	
Decision variables	**Lower bound**	**Upper bound**
Gasification temperature	700 °C	900 °C
Steam to biomass ratio	0	1.5
FT temperature	200 °C	250 °C
FT GHSV	1000 $cm^3/h/g_{cat}$	6000 $cm^3/h/g_{cat}$
FT H2 to CO ratio	1.5	2.5

Both problems are restricted by a set of equality constraints to satisfy the mass and energy balances of the simulation, the defined life cycle costing methodology and the matrix-based life cycle assessment linear equations. Furthermore, there are inequality constraints added by model design specification (i.e., capacity limits, bounds on process variables, etc.).

Both problems are non-linear and coupled. Therefore, the best strategy for finding reasonable solutions is the application of genetic algorithms. eco2des offers different evolutionary algorithms; in this study non-dominated sorting genetic algorithm II, NSGA-II, (K. Deb et al. 2002) was selected for MOOP1. A multi-objective evolutionary algorithm with decomposition, MOEA/D, (Zhang and Li 2007) was selected for MOOP2, because in a preliminary analysis with NSGA-II, the Pareto front has an irregular shape, so MOEA/D may outperform NSGA-II, which also does not scale well with the number of objectives (H. Li and Zhang 2009).

7.3.6. Life cycle interpretation

7.3.6.1. Model inputs

The optimization algorithm of the biorefinery, which produces fuels from biomass in this study, receives the following inputs: biomass input, biomass characteristics, the abovementioned decision variables (see Table 20), plant lifetime, plant capacity factor and construction time.

In this study, corn cob was selected as biomass input. The simulation model needs the following data to characterize the biomass: ultimate analysis (UA) in dry basis, proximate analysis (PA) in dry basis, moisture content and lower heating value (LHV). UA and PA were taken from Phyllis2 database (TNO Biobased and Circular Technologies 2020) and a 14 % of moisture content was assumed. The model allows the introduction of a fixed LHV, but if this value is unknown, the correlation proposed by Souza-Santos (Souza-Santos 2010) is used to estimate it using its UA and PA compositions. Furthermore, Aspen Plus needs a specific heat capacity value in order to define a non-conventional component such as biomass. The polynomial regression, based on the temperature, published by Dupont et al. (2014), were introduced in the simulation.

Finally, 30 years of plant lifetime, 90 % of plant capacity factor and 1.75 years of construction time were assumed in this study.

7.3.6.2. Reference case

In order to establish a baseline scenario, the model was solved using the conclusions of state-of-the-art bibliography (Rafati et al. 2017; Leibbrandt et al. 2013; Dry 2002; Visconti and Mascellaro 2013; Méndez and Ancheyta 2020). Table 21 defines the input variables introduced in the model.

With these operational variables, the biorefinery has an energy efficiency $\left[MW_{fuels+electricity}/MW_{biomass}\right]$ of 47.96 %. Economically, -333.35 M€ was obtained as net present value. Finally, from an environmental point of view a global warming potential of 0.050 kg CO_2-eq. / kWh and a fossil depletion potential of 0.016 kg oil-eq. / kWh were obtained in the aforementioned cradle-to gate approach.

Table 21. Reference case's input variables

Biomass flow	2000 ton/day
Gasification temperature	827 C
Steam to biomass ratio	0.35 wt./wt.
FT Temperature	220 C
FT GHSV	3600 $cm^3/h/g_{cat}$
FT H2 to CO ratio	2.15 mol/mol

Since the NPV is negative using a discount rate of 5 %, a scale-up analysis was carried out using eco2des varying the biomass tones per day (tpd) treated in the plant. The results are shown in Figure 61. On the one hand, environmental impacts are reduced significantly with the increased scale. On the other hand, the NPV has a linear correlation from 1,600 tpd after a minimum value. The NPV becomes positive for a plant which treats 3,185 tpd of biomass (using the reference case's operational variables). However, this value may be prohibitive in terms of biomass harvesting, collection and transport making unfeasible the supply chain management (Mafakheri and Nasiri 2014; Diamantopoulou, Karaoglanoglou, and Koukios 2011). Consequently, a biorefinery which treats 2,800 tpd of biomass was selected for further optimization.

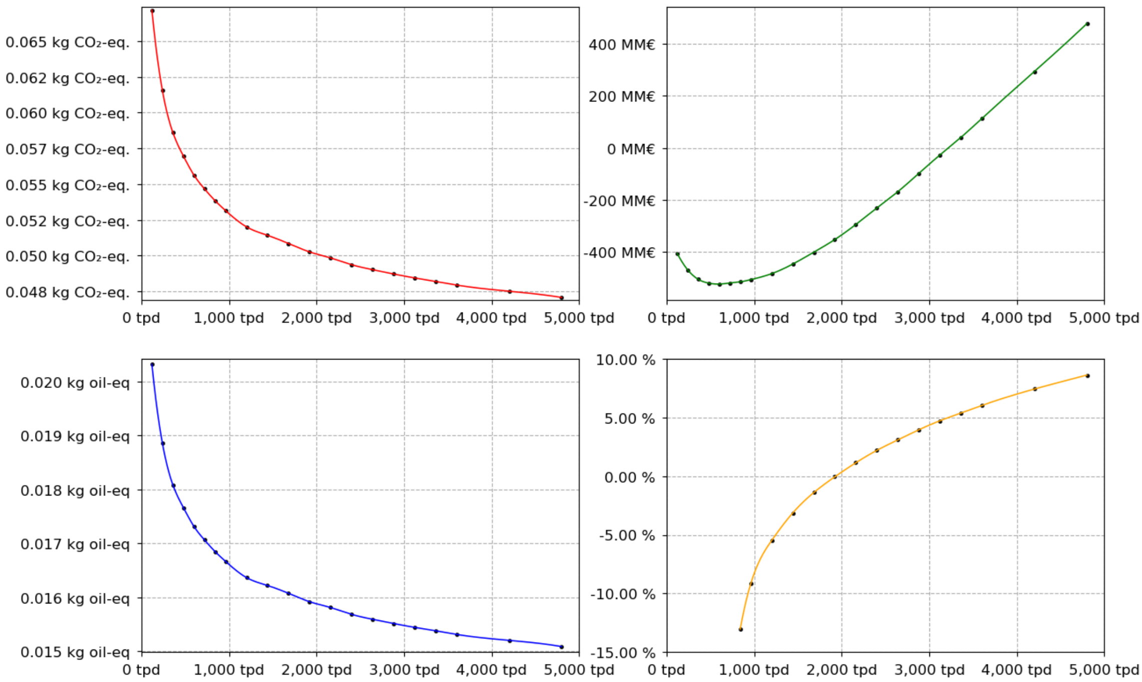

Figure 61. Scale-up analysis (GWP in red, FDP in blue, NPV in green, IRR in orange)

7.3.6.3. Evaluation

All the computational studies are performed on a MSI PS42 8RB-021 laptop with Intel Core i7–8550 U, 4.00 GHz CPU and 16 GB RAM. The CPU time involved in the calculation of each candidate solution is around 69 CPU seconds.

Multi-objective optimization problem 1

The optimization results of MOOP1 are presented in Figure 4. The problem was solved using NSGA-II algorithm: population size, 200; evolutions, 10, crossover probability, 0.95; distribution index for crossover, 10; mutation probability, 0.01; distribution index for mutation, 50.

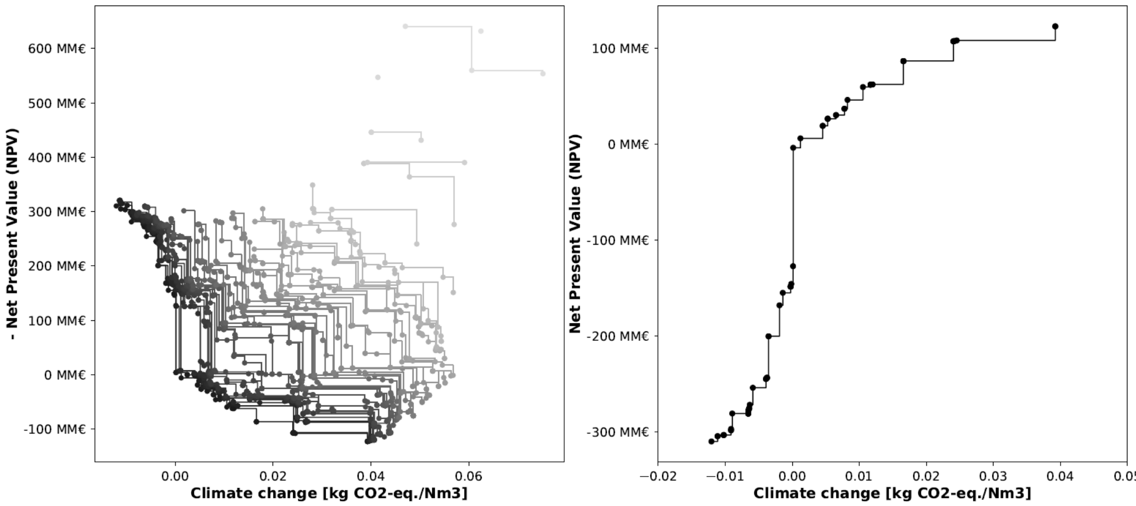

Figure 62. Optimization results for MOOP1: Population evolution (left) and Pareto front (right).

These two objectives are conflicting as anticipated in the preliminary analysis. The Pareto front has a shape similar to a sigmoid, which provides both positive and negative values of the carbon footprint of the process. This phenomenon occurs because the climate change impact is almost determined only by the electricity production in the power plant. If the electricity is enough to cover the climate change burden of the biorefinery value chain upstream activities, a near 0 kg CO_2-eq/Nm^3 impact value is obtained. In this way, if the electricity surplus increases, the climate change impact decreases becoming negative (substituting power from the grid) and if there is no electricity surplus, the impact increases if the electricity demand from the grid increases as well.

On the other hand, the NPV of the plant increases if less surplus electricity is produced, having its optimal value with an electricity production enough to cover the plant demand. This is a consequence from a higher conversion of the biomass into fuels, which have a higher economic value than electricity surplus sales. Nevertheless, the parameter with a higher influence on the economic performance of the biorefinery is the hydrogen production, because, at current market prices, it is the most valuable product. So, in order to obtain maximized values for NPV, the solutions tend to maximize the hydrogen production.

In terms of decision variables, a gasification temperature near to the upper bond favors the minimization of climate change impact because it increases the heat recovered to produce steam for the power plant. On the other hand, a lower gasification temperature increases the conversion of biomass to fuels, because less biomass is oxidized in the gasifier to maintain the desired temperature. This way a higher yield of H_2 and CO is obtained over CO_2 and H_2O. It is worth noting that the lower limit for the gasification temperature in this simulation is determined for the value in which all the carbon content in the biomass is gasified (there is not an excess of char production) based on the result of the thermochemical equilibrium. For the biomass used in this study, this temperature is 716.6 ºC.

Steam to biomass ratio varies from 0.67 to 1.19 in the optimal solutions of the Pareto front, so the injection of steam in the gasifier has a positive benefit for the biorefinery performance. It does not have huge implications in the environmental performance, but better NPV is obtained for values lower than 0.9, since using more steam in the gasifier decreases the thermal power sent to the CHP unit resulting in a lower self-production of electricity. FT temperature does not have a significant implication in the Pareto front shape, but GHSV is a key parameter. GHSV values nearer to the lower bond favors the minimization of the climate change impact, because longer chain hydrocarbons are produced and then more waxes are combusted to produce steam for the power plant. On the other hand, GHSV values nearer to the upper bound increases the H_2 production due to a lower conversion in the FT reactor so they are better to maximize the NPV. Finally, H_2/CO ratio varies from 2.22 to 2.49 (close to the upper bound), so a value higher than the stoichiometric one is beneficial for the plant performance because it also increases the hydrogen production.

The decision variables and objectives of the Pareto front of MOOP1 may be consulted in the APPENDIX A: Decision and objective vectors of the MOOPs.

Multi-objective optimization problem 2

The optimization results of MOOP2 are presented in Figure 63. The problem was solved using MOEA/D algorithm with the Tchebycheff decomposition method (Ma et al. 2018):

Population size, 190; evolutions, 10; size of the weight's neighborhood, 20; crossover parameter, 1; parameter for the differential evolution operator, 0.5; distribution index used by the polynomial mutation, 20.

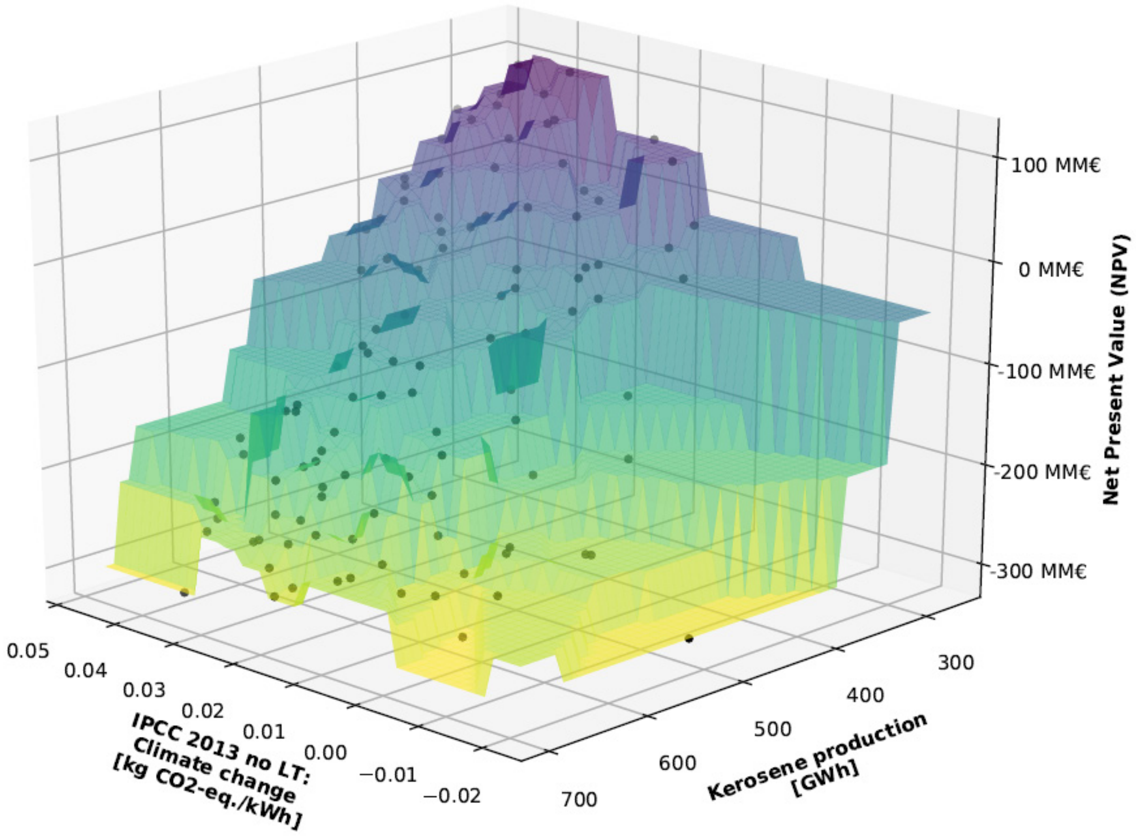

Figure 63. Optimization results for MOOP2: Pareto front.

These three objectives are also conflicting with each other. Global warming impact and NPV have the same behavior than that explained in the previous section. The new objective introduced in this problem, the kerosene production, depends almost exclusively on the GHSV decision variable. GHSV values near the lower bound maximize the kerosene production, while values near to the upper bound minimize it. This occurs because of the high conversion (near 95%) of the wax hydrocracker and the higher conversion and longer chains produced in the FT reactor. However, it resoundingly compromises the economic performance of the biorefinery due to the increase of the hydrogen consumption for wax hydrocracking.

Finally, steam to biomass ratio and H_2/CO ratio affects the kerosene production to a lesser extent. As opposed to the MOOP1, steam to biomass ratios lower than 0.6 benefit the kerosene production, being the maximum kerosene production between 0.1 and 0.6. Furthermore, in this case, a H_2/CO ratio near to the stoichiometric value of 2 maximizes the kerosene production in the biorefinery.

As in the previous case, the decision variables and objectives of the Pareto front of MOOP2 may be consulted in the APPENDIX A: Decision and objective vectors of the MOOPs.

Comparison with reference case

Using the operational variables of Table 21, but with a biomass input of 2,800 tpd, the results obtained for the reference case are as follows the biorefinery has the same energy efficiency of 47.96 %, a NPV of -98.71 MM€, a GWP of 0.049 kg CO2-eq. / kWh and a FDP of 0.016 kg oil-eq. / kWh, i.e., the biorefinery improves its economic performance, although the NPV is still negative.

In order to evaluate the improvements of the multi-objective optimization carried out in the eco2des framework, a set of optimal scenarios are selected from both MOOPs: scenario 1 maximizes the NPV, scenario 2 minimizes the GWP with a NPV ≥ 0, scenario 3 maximizes kerosene production with a NPV ≥ 0 and scenario 4 is a "golden mean" one. Table 22 summarizes the operational variables and results of each scenario and the reference case. Furthermore, the environmental and economic life cycle inventories and financial models for each scenario and the reference system may be consulted in the APPENDIX B: Life cycle inventories of the reference case and the optimal scenarios in the second case study.The results clearly show that the current approaches for biofuels are oriented to the maximization of the amount of liquid fuels in the biorefinery (the highest value of kerosene annual production takes place in the reference case). However, as the results demonstrate, it would make the plant economically unfeasible and the co-production of hydrogen along with liquid fuels is a potential solution. In comparison to the reference cases, it is observed that all optimized scenarios achieve a better economic and environmental performance but reducing the production of kerosene. While scenario 2 achieves the highest environmental impact reduction and scenario 1 achieves the best economic performance, scenario 3 achieves the worst economic and environmental performance but the highest kerosene yield. The average scenario 4 achieves an important improvement of both economic and environmental performance but significantly reducing the production of kerosene. Then, the following observations can be made: (i) the type and quantity of by-products has an important influence on the performance of the integrated biorefinery, with a large influence from market variables (as selling price and environmental footprint) in the optimization results; (ii) the optimization tends to reduce the rate of kerosene production, which is probably caused by the relatively lower price in the market (17.7 EUR/GJ) in comparison to the assumed price of hydrogen (20.8 EUR/GJ), and (iii) the integration of a process simulation model with the inventory for LCA and LCC allows the development of optimized scenarios where an algorithm proposes a set of optimal solutions.

Table 22. Reference case vs optimal scenarios

		Reference case	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Decision variables	Gasification T, °C	827.00	716.59	882.20	734.86	827.06
	steam to biomass (w/w)	0.35	0.67	1.19	0.46	1.05
	FT T, °C	220.00	248.48	222.88	248.42	203.62
	FT GHSV, $cm^3/h/g_{cat}$	3600.00	5973.96	5473.92	4398.44	5217.37
	H2/CO ratio (mol/mol)	2.15	2.49	2.43	2.18	2.49
Energy production, kWh	Hydrogen	850.26	1367.75	1183.26	1060.02	1197.74
	Gasoline	555.83	348.23	324.45	473.74	361.73
	Kerosene	452.1	298.97	272.99	396.53	302.22
	Diesel	242.94	154.92	142.3	210.15	158.1
	Electricity	-27.96	17.58	198.59	-5.73	138.79
	Energy efficiency	47.96%	50.60%	49.08%	49.38%	49.93%
Sustainable performance	NPV, MM€	-98.71	122.7	5.81	3.92	49.34
	GWP, kg CO2-eq. / kWh	0.049	0.039	0.001	0.044	0.015
	FDP, kg oil-eq. / kWh	0.016	0.012	-0.011	0.014	-0.003

7.3.6.4. Conclusions

The optimization of the main design parameters of a biorefinery consisting of biomass gasification and a Fischer Tropsch gas-to-liquid plant has been conducted using eco2des. The results from the optimization showed that the economic performance of the biorefinery can be improved supporting the production of liquid fuels with hydrogen, which is conflicting with the maximization of kerosene production. Also, the environmental performance may be boosted increasing the self-supply of electricity which, in this case, is conflicting with the economic performance and the kerosene production objectives due to the reduction of biomass conversion to fuels. Finally, a comparison with a reference case based on literature values show that the generation of optimal scenarios can boost the understanding of the main interrelation of design parameters and their economic and environmental performance while achieving optimal solutions for the scale-up of a new technology.

8. GENERAL DISCUSSIONS, CONCLUSIONS AND FUTURE WORK

The novel eco-design framework for industrial processes applied in this research has demonstrated its viability for the formulation of optimal scenarios in the process engineering field based on sustainable criteria. It escapes from traditional analysis built with pre-formulated scenarios based on experience which limits the evaluation to some changes in a few topology and operational variables. Thanks to genetic algorithms, thousand scenarios, even millions, can be computed and optimized. This has been demonstrated in two case studies in which the interrelation between design variables and the environmental and economic performance is conflicting and non-linear.

On the one hand, the methanation case study has demonstrated the capabilities of eco2des and how to carry out an eco-design study with this Python tool, highlighting the software's capabilities and its potential for conducting eco-design studies in a holistic way without compromising the simplicity in the implementation. The results have confirmed the tool's effectiveness and its value as a powerful decision support system (DSS) for process engineering. The application of eco2des in early research stages enables the efficient allocation of resources towards projects with genuine sustainable potential. Moreover, the tool's deployment in ongoing process development initiatives can expedite their time-to-value, enhancing their overall sustainability performance.

In the biorefinery case study the capabilities of eco2des have been demonstrated in a complex system, in which literature bases the process design in operational variables that optimize the liquid fuels yield. However, that process design is not optimal in terms of environmental and economic impacts as was demonstrated in the case study development. Consequently, the spreading in the application of an integral methodology based on modelling, LCA, LCC and MOGA, able to generate a potential infinite amount of scenarios, is crucial to accelerate the sustainable time-to-market of novel industrial processes, as well as to ensure that research activities address the main identified hotspots in the scale-up of the technology, defining and optimizing a set of key performance indicators based on not only its technical aspects but also its environmental and economic performance.

The models and simulation used in the eco2des framework are a key parameter for ensuring the accuracy and validity of the results. To develop a rigorous and predictive model is extremely important for the application of this methodology in order to not reach false conclusions. Process simulations, energy systems, supply-chain models, their combination and other complex configurations may be implemented in the framework for their sustainable optimization and scalability. However, inconsistency and problems may occur with systems with an unknown behavior. To ensure the tool reliability is key the expertise of its users in order to develop a rigorous and predictive model while being flexible to converge in the decision space. This is a key challenge and the most time-consuming phase during the P-LCI development.

The main challenge during the eco2des tool development was the lack of a common data interface, which is a huge barrier to achieve the interoperability of the eco-design framework. This lack is not only present between the different integrated frameworks when interchanging inventory data, but also within them. For instance, the LCA framework has a standard that defines the methodology, but there is no agreement around the data model and the environmental flow list used for each background database. Hence, the integration of other databases rather than ecoinvent in the tool is a time-consuming task in order to harmonize the biosphere flows between them and made them compatible for a unique LCA model. There is an initiative that tries to overcome this situation by unifying the different elementary flow lists, the Global LCA Data Access (GLAD) network (GLAD 2023). The primary objective of the GLAD network is to facilitate sustainability-oriented decision-making by promoting enhanced, interoperable, and worldwide availability of LCA datasets, all of them sharing a single biosphere flow list. To achieve this goal, GLAD brings together various stakeholders, including life-cycle dataset providers, to establish a network that fosters collaboration and information exchange.

The same problem happens with process simulation models. Nowadays, each process simulation software has its own data structure which makes difficult to integrate some of them together in a single tool. Therefore, there is also a need for a common interface to exchange simulation data making the development of predictive inventories a straightforward task. In this regard, the CAPE-OPEN standard (van Baten and Pons 2014) is an initiative to achieve interoperability among different software tools used for process simulation. It defines a set of rules and interfaces that enable CAPE (Computer-Aided Process Engineering) applications or components to interoperate with one another, regardless of their origin or programming language. By promoting interoperability, the CAPE-OPEN standard aims to enhance the accuracy and efficiency of process simulations, streamline the development and deployment of CAPE software, and facilitate the exchange of data and models across different domains and applications.

The development of common data schemas and interfaces is key to enable the integration and development of complex methodologies and tools such the one developed during this thesis. eco2des is just another step towards achieving digitalization in the sustainable development within the industry. Digitalization is a critical enabler of sustainable solutions and interoperability, and it is expected to be a key factor in achieving sustainability goals in the future. First, digitalization allows for streamlined data collection, management, and analysis, which is essential for the successful integration of different sustainability-based methods. By enabling the efficient handling of large volumes of data from diverse sources, digital technologies help overcome the challenges associated with data availability and harmonization. Moreover, advanced analytical tools and techniques can provide valuable insights into complex relationships between economic, environmental, and technical factors, thus supporting informed decision-making. Furthermore, digital platforms and tools enable seamless collaboration and communication among stakeholders by fostering cross-disciplinary collaboration and knowledge sharing, digitalization can help break down niches and facilitate the development of holistic solutions that address the multiple dimensions of sustainability. Finally, digitalization can link this new framework with sensors and Internet of Things (IoT) devices providing real-time data to produce real-time predictive inventories that can be used to get continuous insights on process performance, environmental and economic impacts, enabling monitoring and optimization. This real-time allows for dynamic adjustments and improvements that enhance sustainability and overall process efficiency.

To close this chapter, some reflections about future work that may enhance the scope and applications of the eco-design framework and tool for industrial processes are outlined.

First, to address the full spectrum of sustainability dimensions, it is crucial to consider social impacts alongside economic and environmental aspects. The incorporation of Social Life Cycle Assessment (S-LCA) into the integrated methodology can provide a more comprehensive understanding of the social implications of industrial processes. S-LCA evaluates social factors such as labor rights, working conditions, and community relations, thereby enabling a more balanced assessment of sustainability. Future work should explore methods for effectively integrating S-LCA into the framework and eco2des and apply this expanded approach to various case studies.

As abovementioned, eco2des might be applied into real-time solutions through digitalization. By incorporating real-time data from sensors and IoT devices, these integrated methodologies can dynamically adjust to changing conditions and optimize processes more effectively. Future research should focus on developing and implementing digital solutions that leverage real-time data for enhanced decision-making and process optimization.

Furthermore, the current process simulation models, while effective, can be time-consuming and may present a bottleneck in the optimization process. This is not a problem when carrying out early process designs or scaling up studies. However, it is a barrier to implement the methodology in real-time applications in which the optimization problem must be solved as quick as possible. To overcome this limitation, future work should explore the development of AI-driven predictive models based on neural network to produce the P-LCI. These AI-driven models can be trained with simulated data and reproduce the industrial process behavior with greater speed, allowing for more efficient optimization and real-time decision-making.

9. APPENDIX A: Decision and objective vectors of the MOOPs

In this appendix, the decision variables and objective values tables are presented for each one of the multi-objective optimization problems (MOOPs) solved in the case studies. The objective values represent the Pareto front of the problems. For each MOOP, two tables are presented: one with the decision variables and other with the objective values. The row indices of these two tables are related to each other, meaning that the decision variables in the row 1 of the first table resulted in the objective values of the row 1 of the second table. This relationship is exclusive between the pair of tables for a single MOOP.

Table A. 1. First case study, MOOP 1: Decision variables

H_2/CO_2 ratio	Reactor Temperature [C]	Reactor length [m]	Reactor L/D ratio	Power working fluid
4.0347	369.3263	2.3672	7.4280	water
4.0347	369.3263	2.3672	7.4280	water
4.0865	394.3407	2.8074	9.6023	cyclopentane
4.0865	394.3407	2.8074	9.6023	cyclopentane
4.3398	355.6039	3.7199	7.1736	water
4.4621	332.1609	3.3991	5.7908	cyclopentane
4.4621	332.1609	3.3991	5.7908	cyclopentane
4.1511	363.3407	5.6491	9.7213	water
4.4006	355.7108	3.4149	4.6377	cyclopentane
4.3258	372.6467	5.8410	9.7228	water
4.3258	372.6467	5.8410	9.7228	water
4.5229	320.1434	7.0534	8.8117	cyclopentane
4.3525	305.3714	8.5643	8.4436	cyclopentane
4.2390	295.5575	6.3054	4.6991	cyclopentane
4.2390	295.5575	6.3054	4.6991	cyclopentane
4.5129	301.8991	12.4269	9.6358	cyclopentane
4.5129	301.8991	12.4269	9.6358	cyclopentane
4.0163	295.6947	16.0322	8.3680	cyclopentane

Table A. 2. First case study, MOOP 1: Objective values

Storage efficiency [LHV/Electricity]	Climate change [kg CO_2-eq./Nm^3]	Levelized cost of SNG [€/Nm^3]
54.9074	1.6444	1.6951
54.9074	1.6444	1.6951
55.4608	1.6505	1.7926
55.4608	1.6505	1.7926
58.1628	1.1074	1.8928
58.2842	1.1678	2.1561
58.2842	1.1678	2.1561
58.1924	1.1320	2.6994
58.3286	1.1864	2.7315
58.2661	1.1454	2.8438
58.2661	1.1454	2.8438
58.3591	1.2181	4.6553
58.3638	1.2942	7.7291
58.3659	1.3336	9.5147
58.3659	1.3336	9.5147
58.3785	1.4383	14.5413
58.3785	1.4383	14.5413
58.5436	1.9535	36.1375

Table A. 3. First case study, MOOP 2: Decision variables

H_2/CO_2 ratio	Reactor Temperature [C]	Reactor length [m]	Reactor L/D ratio	Power working fluid
4.4510	390.0754	2.5894	5.3640	water
4.4510	390.0754	2.5894	5.3640	water
4.4510	390.0754	2.5894	5.3640	water
4.4510	390.0754	2.5894	5.3640	water
4.4383	397.8995	2.5894	5.3292	cyclopentane
4.4510	389.8766	2.6216	5.3640	cyclopentane
4.4510	389.8766	2.6216	5.3640	cyclopentane
4.4510	389.8766	2.6216	5.3640	cyclopentane
4.4510	389.8766	2.6216	5.3640	cyclopentane
4.4435	379.3340	3.2785	7.4531	cyclopentane
4.4435	379.3340	3.2785	7.4531	cyclopentane
4.4435	379.3340	3.2785	7.4531	cyclopentane

4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.2785	7.4090	cyclopentane
4.4435	379.3340	3.3270	7.2435	cyclopentane
4.5063	343.4695	3.2785	5.5401	cyclopentane
4.5067	319.4885	5.8387	9.2672	cyclopentane
4.5067	319.4885	5.8387	9.2672	cyclopentane
4.5130	319.6406	6.0404	9.1405	cyclopentane
4.5130	319.6406	6.0404	9.1405	cyclopentane
4.5130	319.6406	6.0404	9.1405	cyclopentane
4.5129	316.1545	6.0422	9.0340	cyclopentane
4.5129	316.1545	6.0422	9.0340	cyclopentane
4.5129	316.1545	6.0422	9.0340	cyclopentane
4.5129	316.1545	6.0422	9.0340	cyclopentane
4.5129	316.1545	6.0422	9.0340	cyclopentane
4.5008	319.6406	6.0417	9.0406	cyclopentane
4.5178	315.2413	5.7782	7.9260	cyclopentane
4.5178	315.2413	5.7782	7.9260	cyclopentane
4.5178	315.2413	5.7782	7.9260	cyclopentane
4.5178	319.4989	5.7782	7.8581	cyclopentane
4.5178	319.4989	5.7782	7.8581	cyclopentane
4.5178	319.4989	5.7782	7.8581	cyclopentane
4.5178	319.4989	5.7782	7.8581	cyclopentane
4.5178	319.4989	5.7782	7.8581	cyclopentane
4.4798	303.9806	8.3141	8.1834	cyclopentane
4.4797	303.9806	8.3868	8.0921	cyclopentane
4.4130	307.7826	8.5831	7.4284	cyclopentane
4.4130	307.7826	8.5831	7.4284	cyclopentane
4.4130	307.7826	8.5831	7.4284	cyclopentane
4.0239	364.7179	7.9581	5.5507	cyclopentane
4.0239	358.8071	7.9581	5.5507	cyclopentane
4.0239	358.8071	7.9581	5.5507	cyclopentane

4.0239	358.8071	7.9581	5.5507	cyclopentane
4.0239	358.8071	7.9581	5.5507	cyclopentane
4.0239	358.8071	7.9581	5.5507	cyclopentane
4.0239	357.8110	7.9581	5.5507	cyclopentane
4.0239	357.8110	7.9581	5.5507	cyclopentane
4.0239	344.3982	8.3501	5.9055	cyclopentane
4.0307	342.1860	8.2113	5.5507	cyclopentane
4.0085	319.2267	11.7594	9.1892	cyclopentane
4.0085	319.2267	11.7594	9.1892	cyclopentane
4.0085	319.2267	11.7594	9.1892	cyclopentane
4.0087	319.2267	11.7596	9.1833	cyclopentane
4.0087	319.2267	11.7596	9.1833	cyclopentane
4.0087	319.2267	11.7596	9.1833	cyclopentane
4.0239	318.2545	12.2395	8.7869	cyclopentane
4.0128	312.3117	12.1813	8.6894	cyclopentane
4.0128	312.3117	12.1813	8.6894	cyclopentane
4.0128	312.3117	12.1813	8.6894	cyclopentane
4.0482	317.0975	12.2830	6.1044	cyclopentane
4.0482	317.0975	12.2830	6.1044	cyclopentane
4.0482	317.0975	12.2830	6.1044	cyclopentane
4.0105	285.4899	16.8270	7.9169	cyclopentane
4.0105	285.4899	16.8270	7.9169	cyclopentane
4.0105	285.4899	16.8270	7.9169	cyclopentane
4.0105	285.4899	16.8270	7.9169	cyclopentane
4.0105	285.4899	16.8270	7.9169	cyclopentane

Table A. 4. First case study, MOOP 2: Objective values

Storage efficiency [LHV/Electricity]	Levelized cost of SNG [€/Nm3]
57.9538	1.5188
57.9538	1.5188
57.9538	1.5188
57.9538	1.5188
58.2561	1.6238
58.2742	1.6418
58.2752	1.6421
58.2752	1.6421
58.2752	1.6421

	58.2939	1.6560
	58.2939	1.6560
	58.2939	1.6560
	58.2940	1.6635
	58.2940	1.6635
	58.2948	1.6638
	58.2948	1.6638
	58.2948	1.6638
	58.2948	1.6638
	58.2948	1.6638
	58.2948	1.6638
	58.2950	1.7216
	58.3415	2.1291
	58.3582	3.0659
	58.3582	3.0659
	58.3588	3.3087
	58.3588	3.3087
	58.3588	3.3088
	58.3625	3.3579
	58.3625	3.3579
	58.3625	3.3579
	58.3625	3.3579
	58.3625	3.3579
	58.3632	3.3581
	58.3640	3.6295
	58.3640	3.6296
	58.3640	3.6296
	58.3736	3.6632
	58.3736	3.6632
	58.3736	3.6632
	58.3736	3.6632
	58.3736	3.6632
	58.3779	7.4224
	58.4124	7.6854
	58.4754	9.2935
	58.4754	9.2935
	58.4754	9.2935

58.4980	12.2621
58.5053	12.2632
58.5053	12.2632
58.5053	12.2632
58.5054	12.2634
58.5054	12.2634
58.5064	12.2635
58.5064	12.2635
58.5185	12.4602
58.5228	13.1981
58.5407	14.1606
58.5407	14.1606
58.5407	14.1606
58.5409	14.1747
58.5409	14.1749
58.5409	14.1749
58.5431	16.7666
58.5475	16.9480
58.5475	16.9480
58.5475	16.9480
58.5476	30.6741
58.5476	30.6741
58.5476	30.6741
58.5586	44.8005
58.5586	44.8005
58.5586	44.8005
58.5586	44.8005
58.5586	44.8005

Table A. 5. Second case study, MOOP 1: Decision variables

Gasification temperature [C]	Steam ratio	FT temperature [C]	GHSV [$cm^3/h/g_{cat}$]	H_2/CO ratio
894.7401	1.1545	225.1900	1284.9049	2.2717
893.3914	1.1367	245.0662	1401.5226	2.2669
893.3914	1.1221	245.0662	1401.5226	2.2669
899.9780	1.1124	203.9911	1937.5181	2.2206
882.3435	1.1104	210.2341	1117.2984	2.2683

893.2488	1.1906	204.7159	1987.3337	2.4048
899.9780	1.1124	242.8592	2233.6705	2.2206
899.9780	1.1124	242.5402	2233.6705	2.2206
899.9780	1.1124	242.5402	2233.6705	2.2206
896.6705	1.1124	246.0000	2231.4333	2.2214
895.2174	1.1124	242.5402	2232.3695	2.2206
895.2174	1.1124	240.1155	2238.1544	2.2206
894.6401	1.1367	204.9330	2279.3652	2.2765
862.1701	1.1448	216.6584	1321.1810	2.4258
854.1394	1.1169	205.7137	1182.7468	2.4315
854.1394	1.1169	205.5521	1182.7468	2.4390
892.4473	1.1294	248.1684	2944.3479	2.2547
895.3445	1.1353	227.5069	3299.8002	2.2702
895.3445	1.1349	227.2694	3429.6463	2.2704
899.8559	1.1121	238.5064	3529.4478	2.2195
899.8559	1.1121	240.9545	3531.2258	2.2261
897.6972	1.1121	240.9545	3531.2258	2.2261
896.1059	1.1293	225.9191	3729.8707	2.2717
893.2281	1.1906	240.2226	5490.7321	2.4116
882.2050	1.1906	222.8835	5473.9216	2.4254
892.7710	1.1221	245.0662	5823.5605	2.2669
871.3326	1.1411	239.9401	5566.3832	2.4119
871.7761	1.1374	242.2331	5664.3458	2.4755
867.9313	1.1105	238.7448	5675.1425	2.3824
854.2013	1.1184	247.7539	5579.8926	2.4755
858.5603	1.0833	238.7359	5915.9003	2.3811
852.9095	1.0833	204.9938	5915.9003	2.3811
852.9095	1.0796	205.7075	5915.9003	2.3862
827.8595	1.0347	205.9328	5918.4344	2.4470
827.7671	1.0347	205.9328	5918.4344	2.4470
803.2993	0.9277	221.6465	5933.0778	2.4248
804.1318	0.9276	221.6465	5950.9769	2.4265
804.1318	0.9276	216.5559	5965.3781	2.4258
803.2993	0.9277	206.1302	5985.0818	2.4248
716.5899	0.6697	248.4771	5973.9612	2.4867

Table A. 6. Second case study, MOOP 1: Objective values

Climate change [kg CO_2-eq./Nm^3]	Net Present Value [M€]
-0.0121	-310.3130
-0.0111	-304.8263
-0.0102	-303.6305
-0.0091	-298.6243
-0.0091	-297.2574
-0.0090	-281.1050
-0.0066	-281.0915
-0.0066	-281.0908
-0.0066	-281.0839
-0.0065	-277.4830
-0.0065	-276.0510
-0.0064	-275.7139
-0.0063	-272.0147
-0.0059	-254.2465
-0.0039	-245.0640
-0.0038	-243.8788
-0.0035	-200.5327
-0.0019	-168.2093
-0.0014	-155.1433
-0.0002	-148.6674
-0.0002	-148.2321
-0.0001	-145.8616
0.0001	-127.3635
0.0001	-3.7183
0.0012	6.1130
0.0045	19.1616
0.0053	26.5994
0.0065	30.4053
0.0078	37.0382
0.0082	46.2664
0.0105	59.7003
0.0117	62.1759
0.0120	62.3919
0.0166	86.6426
0.0166	86.8085

0.0240	107.4087
0.0241	107.5744
0.0242	107.7674
0.0245	108.3397
0.0392	123.0537

Table A. 7. Second case study, MOOP 2: Decision variables

Gasification temperature [C]	Steam ratio	FT temperature [C]	GHSV [cm3/h/g_{cat}]	H_2/CO ratio
897.0497	0.8468	241.4349	1587.0459	2.0115
821.2784	0.1501	235.9251	1189.6216	1.6665
895.7811	1.3319	200.3812	1014.4796	2.4889
771.8997	0.3891	204.8425	1008.7655	1.6496
838.8835	0.4999	232.8880	1128.8324	1.9146
866.9177	0.7273	229.3616	1675.4964	1.9930
858.2530	0.8605	223.0046	1046.7529	2.2015
856.7325	1.0060	200.7140	1029.4445	2.2800
884.8647	0.8438	223.8600	2086.8042	2.0762
716.0057	0.4072	240.0724	1138.8100	1.9634
821.6836	0.5970	200.7790	1593.9655	1.8344
806.7882	0.5970	226.1587	1193.1093	1.9021
885.3390	1.1556	234.3856	2340.1549	2.4465
880.6393	1.1544	223.4402	2312.8222	2.4374
827.5668	0.6630	228.3881	1812.9915	1.8730
756.6747	0.4123	244.0062	1058.8132	2.1494
725.9682	0.3731	228.3621	1493.7958	1.9989
860.6658	1.0196	214.6662	1815.3192	2.3935
705.6649	0.3883	205.3666	1782.6236	1.7862
822.7817	0.1054	249.5571	1111.7636	2.1282
840.3295	0.2003	246.1868	1750.6271	2.0426
861.6922	1.0142	229.8802	2018.3133	2.3632
866.0325	0.8147	224.2675	2133.9260	2.1856
818.9609	0.5878	249.2791	1947.6650	1.8795
775.8297	0.5749	246.0030	1275.6962	2.1440
753.6879	0.4293	244.2159	1987.1177	1.8181
822.5051	0.1432	249.4087	1506.5940	2.1834
743.3829	0.4608	208.8245	1007.4689	2.2733

795.8541	0.6917	243.3636	1845.1004	2.1300
875.8108	0.9715	227.9074	2785.9011	2.2164
827.3663	0.8674	201.3894	1869.7308	2.4271
713.1821	0.5157	223.4587	1768.4320	2.1000
715.1859	0.4957	238.9427	1968.0498	2.0299
897.0537	1.1109	208.5323	3154.1559	2.3608
899.9783	0.0916	246.8539	1004.5715	2.3053
848.4478	0.1123	239.0791	2078.8080	2.1863
732.0166	0.4936	206.9996	1803.0708	2.2809
802.0777	0.8355	203.9168	1239.6332	2.4952
767.8395	0.6594	245.1680	1246.6683	2.4117
700.6157	0.5082	217.5841	1620.6897	2.3499
821.0353	0.1240	225.1771	1406.4343	2.4543
708.5909	0.5439	200.0289	1427.8134	2.4582
798.1693	0.8861	246.4960	2112.5352	2.4620
750.0344	0.7362	241.5741	1781.4218	2.3784
701.6950	0.4747	231.8140	2365.9929	2.0611
809.9865	0.7859	232.8601	2573.8235	2.1973
842.7936	0.9373	225.5965	2918.2792	2.2244
898.3067	1.0688	215.8495	3571.2686	2.4171
858.5519	0.9523	233.0584	3167.8783	2.5000
898.3506	0.0496	248.7027	1861.8197	2.4512
880.1871	0.0128	237.9043	1230.5232	2.4990
751.3750	0.5960	206.9466	2381.9407	2.4231
899.3251	0.0538	248.9344	1919.0986	2.4729
758.0723	0.6833	211.8962	2404.0843	2.4606
780.7787	0.7689	239.5503	2547.0639	2.4712
714.3598	0.4244	245.1264	2888.1031	2.0399
742.7110	0.6231	204.3962	2828.0418	2.2256
753.8025	0.7516	207.1941	2700.4038	2.4374
703.9797	0.5588	244.9041	2692.4296	2.3889
713.7859	0.5371	204.0619	2812.3208	2.3508
812.8534	0.9000	204.6712	3237.7066	2.4568
765.8421	0.6030	219.2816	2988.1225	2.4349
806.5384	0.9805	231.4794	3282.9623	2.4935
846.8930	0.9846	222.7968	3744.6235	2.4301
828.7019	0.8417	243.6457	3669.2091	2.2690

727.3256	0.6542	238.5339	3000.3966	2.4869
845.7063	1.0007	212.9680	3878.3653	2.3208
824.0411	0.8801	236.2372	3711.2340	2.3678
816.8885	0.6732	200.0551	3647.1513	2.4995
730.3789	0.4384	200.5206	3554.5518	2.2060
884.5517	1.0729	241.7134	4516.4212	2.4038
820.9504	0.8660	223.5611	3853.6634	2.3401
825.8977	0.9987	217.2242	3879.8444	2.4831
752.9183	0.5346	223.0373	3592.7949	2.3498
848.0225	0.9599	207.0000	4180.3717	2.2598
835.2156	0.9830	205.0138	4052.0648	2.4195
801.2780	0.7155	214.1235	3812.9781	2.4813
745.3465	0.4213	224.8536	3917.3279	2.4458
807.9825	0.6228	225.1908	4024.0657	2.1325
877.6985	1.0483	236.3226	4733.7606	2.4863
814.1135	0.7287	209.0377	4125.3422	2.3064
811.1490	0.6669	215.4067	4131.2099	2.4442
730.6032	0.4627	207.9660	3958.5711	2.3496
802.0083	0.7021	229.3214	4210.6764	2.0397
877.0698	1.0772	203.5844	5079.6399	2.4823
742.1230	0.5188	228.3240	4120.2791	2.3831
825.9557	0.9149	246.1285	4400.3650	2.3864
865.8620	0.8530	205.7861	4938.6449	2.0617
804.2389	0.8136	249.9829	4303.1778	2.2503
864.4186	0.8829	203.1694	5039.6124	2.4462
734.8597	0.4631	248.4229	4398.4377	2.1790
712.2530	0.4702	249.7221	4380.8698	2.4999
732.2168	0.6041	226.4406	4360.8199	2.4975
789.3128	0.7144	226.1786	4647.2782	2.2060
825.6955	0.8376	217.4192	4950.3407	2.3279
764.6111	0.5140	227.7857	5016.8887	2.1887
815.7244	0.6931	211.1318	5123.9718	2.1547
827.0553	1.0518	203.6197	5217.3681	2.4934
862.4008	0.9555	228.3376	5845.1276	2.4953
753.8760	0.5515	210.7781	5201.0611	1.9447
749.0057	0.5042	232.1087	5483.9037	2.2060
805.9094	0.7447	215.0621	5274.0041	2.0869

811.8427	0.7656	224.1547	5354.5593	2.1981
793.9440	0.6439	224.6449	5415.5762	2.1777
803.0497	0.6391	231.1121	5605.8501	2.2118
799.9394	0.7488	201.7796	5637.3134	2.3112
800.4882	0.7736	213.2998	5972.5852	2.3190
758.5241	0.6668	246.8006	5824.4347	2.3999

Table A. 8. Second case study, MOOP 2: Objective values

Climate change [kg CO_2-eq./Nm^3]	Net Present Value [M€]	Kerosene production [GWh]
0.0004	-303.9744	616.9604
0.0333	-298.4664	696.4275
-0.0211	-293.0285	523.8954
0.0191	-276.6811	690.7723
0.0187	-272.8148	674.4935
0.0078	-270.3033	632.2970
0.0037	-267.7772	623.3830
-0.0024	-263.6057	598.8822
0.0058	-263.2330	580.8296
0.0205	-252.6499	686.5197
0.0112	-252.2358	662.3499
0.0114	-252.0493	674.0335
-0.0043	-246.2323	514.5592
-0.0041	-244.5782	518.8725
0.0093	-241.5848	642.0488
0.0253	-239.7701	673.5972
0.0250	-238.4747	669.9260
0.0011	-238.3574	567.6656
0.0211	-237.3155	663.7547
0.0311	-237.0855	684.9226
0.0333	-235.3102	661.6707
0.0014	-234.8707	561.6611
0.0103	-234.7034	578.9818
0.0150	-229.3390	636.1263
0.0169	-221.2694	661.3046
0.0218	-220.2254	646.8835
0.0333	-218.5397	663.7368
0.0247	-217.5058	654.7841

0.0128	-202.1247	628.2401
0.0086	-198.0880	490.9295
0.0108	-194.9512	581.5432
0.0194	-194.2438	640.1133
0.0207	-190.0293	631.1462
0.0018	-186.2051	435.4309
0.0249	-185.0199	652.1513
0.0343	-183.4202	628.0286
0.0252	-180.7736	622.5202
0.0133	-178.8914	589.4914
0.0190	-178.6686	618.6504
0.0233	-172.2144	621.4956
0.0348	-167.9800	628.0157
0.0235	-164.5967	614.1636
0.0110	-159.1619	570.1760
0.0142	-157.6842	606.8290
0.0251	-155.4649	591.7676
0.0158	-152.0736	545.3428
0.0120	-150.7604	486.9858
0.0074	-144.1309	398.5968
0.0178	-140.1822	454.3489
0.0273	-131.8133	616.6050
0.0280	-130.6785	622.6915
0.0260	-129.7768	566.5985
0.0279	-127.9819	611.2754
0.0224	-123.5809	559.8235
0.0201	-121.7923	542.8714
0.0329	-118.5427	540.3369
0.0248	-101.9448	532.5891
0.0205	-99.1360	531.9987
0.0280	-97.5969	538.6487
0.0301	-96.2768	530.7823
0.0201	-91.0927	461.3626
0.0315	-88.4843	508.3103
0.0156	-80.8608	453.6196
0.0161	-74.3704	400.7830
0.0249	-68.6506	418.8079

0.0274	-68.1586	504.1442
0.0139	-61.7233	388.1078
0.0233	-59.5410	414.4569
0.0365	-58.0475	432.7492
0.0406	-55.8405	467.2357
0.0089	-49.3257	329.8660
0.0248	-46.5065	403.3635
0.0162	-43.7488	393.6517
0.0381	-43.7198	455.3552
0.0173	-39.6491	365.5320
0.0174	-39.2022	378.1560
0.0346	-36.7372	418.9343
0.0457	-33.0396	429.7797
0.0372	-28.7812	403.6777
0.0128	-27.8966	319.5700
0.0346	-23.5651	389.4336
0.0394	-20.7324	392.9768
0.0435	-19.3255	428.2752
0.0326	-10.6483	385.7774
0.0119	-9.4582	298.7978
0.0422	-3.4022	411.8783
0.0221	-1.5888	357.6015
0.0248	-0.6957	315.8825
0.0276	2.7454	373.6545
0.0278	3.1734	311.8168
0.0444	3.9401	396.5397
0.0448	10.2313	394.3175
0.0397	21.9834	390.5543
0.0355	25.9178	357.4583
0.0292	31.6437	325.5297
0.0459	36.8787	347.9916
0.0385	41.9001	323.0270
0.0150	49.5230	302.1941
0.0227	51.4365	269.9852
0.0423	58.8736	338.7758
0.0468	59.1727	324.8970
0.0334	62.0717	314.3104

	0.0332	64.6235	308.4002
	0.0419	67.5492	313.9738
	0.0430	74.6290	302.7044
	0.0366	82.8104	297.7406
	0.0348	102.9316	281.3089
	0.0406	106.3905	299.9317

10. APPENDIX B: Life cycle inventories of the reference case and the optimal scenarios in the second case study

In this appendix, the environmental and economic inventories of the reference case and the optimal scenarios of the biofuels production case study (Section 7.3.6.3) are detailed.

Table B. 1. Biosphere inventory data of the reference case (FU: 1 kWh of biofuels)

Elementary flow	Amount	Unit
Water, to air	0.036254752	m^3
Carbon dioxide, non-fossil, to non-urban air or from high stacks	0.509664237	kg
Carbon monoxide, non-fossil, to non-urban air or from high stacks	8.87045E-09	kg
Oxygen, to in air	0.214202225	kg
Nitrogen, to in air	-0.00209022	kg
Nitrogen oxides, to non-urban air or from high stacks	8.62264E-06	kg
Hydrochloric acid, to air	1.60113E-09	kg
Chlorine, to non-urban air or from high stacks	1.12252E-17	kg
Sulfur dioxide, to non-urban air or from high stacks	0.000698421	kg
Sulfur trioxide, to non-urban air or from high stacks	2.11545E-06	kg
Methanol, non-urban air or from high stacks	0.000428115	kg
Water, cooling, unspecified natural origin, to in water	0.000291132	m^3

Table B. 2. Technosphere inventory data of the reference case (FU: 1 kWh of biofuels)

Activity	Amount	Unit
market for wood chips, wet, measured as dry mass	0.425188303	kg
market for wood ash mixture, pure	-0.011981264	kg
market for dolomite	0.005551047	kg
market for zeolite, powder	0.001136934	kg
market for waste zeolite	-0.001136934	kg
market for silica sand	0.006885112	kg
market for sulfuric acid	0	kg
market for sodium hydroxide, without water, in 50% solution state	0.000175285	kg
market for zinc oxide	4.52618E-07	kg
synthetic gas factory construction	5.96929E-09	unit

air separation facility construction	6.27511E-09	unit
water production, completely softened	0.016791552	kg
market for water, decarbonized	0.534317076	kg
market for wastewater, from residence	-0.000562365	m^3
petroleum refinery construction	3.56024E-10	unit
gas power plant construction, 100MW electrical	2.04337E-14	unit
market for methanol	0.000428115	kg
market for cobalt	1.09349E-06	kg
market for molybdenum	1.88712E-07	kg
market for magnetite	1.45707E-07	kg
market for chromium oxide, flakes	1.9637E-08	kg
market for magnesium oxide	3.9274E-10	kg
market for nickel, 99.5%	6.18629E-08	kg
market for platinum	2.38362E-10	kg
market for selenium	2.38362E-10	kg
market for aluminum oxide, non-metallurgical	6.82993E-06	kg
market for inert waste, for final disposal	-0.012436159	kg
market for electricity, medium voltage	0.013306066	kWh
electricity production, natural gas, combined cycle power plant	0	kWh

Table B. 3. Biosphere inventory data of the optimal scenario 1 (FU: 1 kWh of biofuels)

Elementary flow	Amount	Unit
Water, to air	0.038216457	m^3
Carbon dioxide, non-fossil, to non-urban air or from high stacks	0.546958447	kg
Carbon monoxide, non-fossil, to non-urban air or from high stacks	4.78423E-09	kg
Oxygen, to in air	0.210930198	kg
Nitrogen, to in air	-0.001992338	kg
Nitrogen oxides, to non-urban air or from high stacks	9.21184E-06	kg
Hydrochloric acid, to air	1.55072E-09	kg
Chlorine, to non-urban air or from high stacks	6.62209E-18	kg
Sulfur dioxide, to non-urban air or from high stacks	0.00067629	kg
Sulfur trioxide, to non-urban air or from high stacks	2.04568E-06	kg
Methanol, non-urban air or from high stacks	0.000457872	kg
Water, cooling, unspecified natural origin, to in water	0.000339474	m^3

Table B. 4. Technosphere inventory data of the optimal scenario 1 (FU: 1 kWh of biofuels)

Activity	Amount	Unit
market for wood chips, wet, measured as dry mass	0.4117136	kg
market for wood ash mixture, pure	-0.011601564	kg
market for dolomite	0.005155847	kg
market for zeolite, powder	0.001055992	kg
market for waste zeolite	-0.001055992	kg
market for silica sand	0.006394935	kg
market for sulfuric acid	0	kg
market for sodium hydroxide, without water, in 50% solution state	0.000169647	kg
market for zinc oxide	4.26351E-07	kg
synthetic gas factory construction	5.78012E-09	unit
air separation facility construction	6.04226E-09	unit
water production, completely softened	0.020396939	kg
market for water, decarbonized	0.627739608	kg
market for wastewater, from residence	-0.000608378	m^3
petroleum refinery construction	3.56526E-10	unit
gas power plant construction, 100MW electrical	2.53842E-14	unit
market for methanol	0.000457872	kg
market for cobalt	6.91753E-07	kg
market for molybdenum	1.49164E-07	kg
market for magnetite	3.72894E-09	kg
market for chromium oxide, flakes	5.02553E-10	kg
market for magnesium oxide	1.00511E-11	kg
market for nickel, 99.5%	5.50591E-08	kg
market for platinum	1.43943E-10	kg
market for selenium	1.43943E-10	kg
market for aluminum oxide, non-metallurgical	4.52836E-06	kg
market for inert waste, for final disposal	-0.011550782	kg
market for electricity, medium voltage	0	kWh
electricity production, natural gas, combined cycle power plant	-0.008282325	kWh

Table B. 5. Biosphere inventory data of the optimal scenario 2 (FU: 1 kWh of biofuels)

Elementary flow	Amount	Unit
Water, to air	0.036932252	m^3

Carbon dioxide, non-fossil, to non-urban air or from high stacks	0.6255548	kg
Carbon monoxide, non-fossil, to non-urban air or from high stacks	5.52613E-09	kg
Oxygen, to in air	0.270336539	kg
Nitrogen, to in air	-0.002341761	kg
Nitrogen oxides, to non-urban air or from high stacks	8.8884E-06	kg
Hydrochloric acid, to air	1.74987E-09	kg
Chlorine, to non-urban air or from high stacks	1.88027E-17	kg
Sulfur dioxide, to non-urban air or from high stacks	0.000763122	kg
Sulfur trioxide, to non-urban air or from high stacks	2.31688E-06	kg
Methanol, non-urban air or from high stacks	0.000529474	kg
Water, cooling, unspecified natural origin, to in water	0.00055493	m^3

Table B. 6. Technosphere inventory data of the optimal scenario 2 (FU: 1 kWh of biofuels)

Activity	Amount	Unit
market for wood chips, wet, measured as dry mass	0.464579523	kg
market for wood ash mixture, pure	-0.013091258	kg
market for dolomite	0.006643779	kg
market for zeolite, powder	0.001360742	kg
market for waste zeolite	-0.001360742	kg
market for silica sand	0.008240458	kg
market for sulfuric acid	0	kg
market for sodium hydroxide, without water, in 50% solution state	0.000191616	kg
market for zinc oxide	5.46311E-07	kg
synthetic gas factory construction	6.52231E-09	unit
air separation facility construction	7.7484E-09	unit
water production, completely softened	0.036376651	kg
market for water, decarbonized	0.953604579	kg
market for wastewater, from residence	-0.000954875	m^3
petroleum refinery construction	3.41641E-10	unit
gas power plant construction, 100MW electrical	4.52536E-14	unit
market for methanol	0.000529474	kg
market for cobalt	6.92517E-07	kg
market for molybdenum	1.36429E-07	kg
market for magnetite	1.16756E-08	kg
market for chromium oxide, flakes	1.57353E-09	kg
market for magnesium oxide	3.14705E-11	kg

market for nickel, 99.5%	4.78014E-08	kg
market for platinum	1.51538E-10	kg
market for selenium	1.51538E-10	kg
market for aluminum oxide, non-metallurgical	4.4364E-06	kg
market for inert waste, for final disposal	-0.014884236	kg
market for electricity, medium voltage	0	kWh
electricity production, natural gas, combined cycle power plant	-0.103463367	kWh

Table B. 7. Biosphere inventory data of the optimal scenario 3 (FU: 1 kWh of biofuels)

Elementary flow	Amount	Unit
Water, to air	0.039043009	m^3
Carbon dioxide, non-fossil, to non-urban air or from high stacks	0.520864069	kg
Carbon monoxide, non-fossil, to non-urban air or from high stacks	6.48822E-09	kg
Oxygen, to in air	0.210191682	kg
Nitrogen, to in air	-0.002020227	kg
Nitrogen oxides, to non-urban air or from high stacks	9.3789E-06	kg
Hydrochloric acid, to air	1.57202E-09	kg
Chlorine, to non-urban air or from high stacks	6.68892E-18	kg
Sulfur dioxide, to non-urban air or from high stacks	0.000685599	kg
Sulfur trioxide, to non-urban air or from high stacks	2.07738E-06	kg
Methanol, non-urban air or from high stacks	0.000434189	kg
Water, cooling, unspecified natural origin, to in water	0.000310663	m^3

Table B. 8. Technosphere inventory data of the optimal scenario 3 (FU: 1 kWh of biofuels)

Activity	Amount	Unit
market for wood chips, wet, measured as dry mass	0.417382598	kg
market for wood ash mixture, pure	-0.011761309	kg
market for dolomite	0.005052323	kg
market for zeolite, powder	0.001034788	kg
market for waste zeolite	-0.001034788	kg
market for silica sand	0.006266531	kg
market for sulfuric acid	0	kg
market for sodium hydroxide, without water, in 50% solution state	0.000172014	kg
market for zinc oxide	4.1698E-07	kg
synthetic gas factory construction	5.85971E-09	unit

air separation facility construction	6.02145E-09	unit
water production, completely softened	0.018159661	kg
market for water, decarbonized	0.518301666	kg
market for wastewater, from residence	-0.000523854	m^3
petroleum refinery construction	3.77896E-10	unit
gas power plant construction, 100MW electrical	2.23997E-14	unit
market for methanol	0.000434189	kg
market for cobalt	9.63717E-07	kg
market for molybdenum	1.82285E-07	kg
market for magnetite	6.09098E-08	kg
market for chromium oxide, flakes	8.20887E-09	kg
market for magnesium oxide	1.64177E-10	kg
market for nickel, 99.5%	6.40099E-08	kg
market for platinum	1.99007E-10	kg
market for selenium	1.99007E-10	kg
market for aluminum oxide, non-metallurgical	6.1288E-06	kg
market for inert waste, for final disposal	-0.011318853	kg
market for electricity, medium voltage	0.002657437	kWh
electricity production, natural gas, combined cycle power plant	0	kWh

Table B. 9. Biosphere inventory data of the optimal scenario 4 (FU: 1 kWh of biofuels)

Elementary flow	Amount	Unit
Water, to air	0.035808124	m^3
Carbon dioxide, non-fossil, to non-urban air or from high stacks	0.585082054	kg
Carbon monoxide, non-fossil, to non-urban air or from high stacks	5.03883E-09	kg
Oxygen, to in air	0.243813589	kg
Nitrogen, to in air	-0.00220656	kg
Nitrogen oxides, to non-urban air or from high stacks	8.56597E-06	kg
Hydrochloric acid, to air	1.6666E-09	kg
Chlorine, to non-urban air or from high stacks	1.558E-17	kg
Sulfur dioxide, to non-urban air or from high stacks	0.000726575	kg
Sulfur trioxide, to non-urban air or from high stacks	2.20624E-06	kg
Methanol, non-urban air or from high stacks	0.000494928	kg
Water, cooling, unspecified natural origin, to in water	0.000470016	m^3

Table B. 10. Technosphere inventory data of the optimal scenario 4 (FU: 1 kWh of biofuels)

Activity	Amount	Unit
market for wood chips, wet, measured as dry mass	0.442330718	kg
market for wood ash mixture, pure	-0.012464315	kg
market for dolomite	0.006419919	kg
market for zeolite, powder	0.001314892	kg
market for waste zeolite	-0.001314892	kg
market for silica sand	0.007962799	kg
market for sulfuric acid	0	kg
market for sodium hydroxide, without water, in 50% solution state	0.000182361	kg
market for zinc oxide	5.26849E-07	kg
synthetic gas factory construction	6.20996E-09	unit
air separation facility construction	7.06901E-09	unit
water production, completely softened	0.030214043	kg
market for water, decarbonized	0.829013884	kg
market for wastewater, from residence	-0.000827045	m^3
petroleum refinery construction	3.32072E-10	unit
gas power plant construction, 100MW electrical	3.75905E-14	unit
market for methanol	0.000494928	kg
market for cobalt	7.22782E-07	kg
market for molybdenum	1.40086E-07	kg
market for magnetite	5.1084E-09	kg
market for chromium oxide, flakes	6.88464E-10	kg
market for magnesium oxide	1.37693E-11	kg
market for nickel, 99.5%	4.83817E-08	kg
market for platinum	1.60907E-10	kg
market for selenium	1.60907E-10	kg
market for aluminum oxide, non-metallurgical	4.61064E-06	kg
market for inert waste, for final disposal	-0.014382718	kg
market for electricity, medium voltage	0	kWh
electricity production, natural gas, combined cycle power plant	-0.068987995	kWh

Table B. 11. CAPEX of the reference case

Equipment and Installation	Biomass storage, preparation and feed	17,949,017.53 €
	Biomass air dryer	170,014.25 €
	CFB gasifier, gas cooling and gas cleaning	181,907,154.74 €
	ASU with O2 and N2 compressors	156,611,845.55 €
	Rectisol unit	66,006,327.19 €
	Water gas shift reactor	1,020,553.62 €
	ATR Reactor	15,893,826.18 €
	PSA	18,241,223.10 €
	Fisher-Tropsch slurry reactor	74,592,243.26 €
	Distillation recovery plant	17,326,967.50 €
	Wax hydrocracker	23,074,679.01 €
	Naphtha hydrotreater	2,465,940.13 €
	Kerosene hydrotreater	5,447,159.79 €
	Diesel hydrotreater	9,917,742.99 €
	Isomerization unit	4,336,686.42 €
	Heavy naphtha reformer	25,969,036.92 €
	Heat recovery steam generator	21,899,287.70 €
	Steam cycle	6,784,948.50 €
	Auxiliary compressors	12,858,441.03 €
	Auxiliary pumps	35,575.25 €
	Co/Al2O3	510,952.77 €
	Co/Mo/Al2O3	38,227.14 €
	Ni/Mo/Al2O3	58,507.50 €
	Fe/Cr/Mg	26,353.49 €
	Pt/Re/Al2O3	284,301.78 €
ISBL		663,427,013.35 €
OSBL		218,755,219.85 €
Engineering and Design		279,182,264.34 €
Contingency		88,126,389.05 €
TOTAL		1,249,490,886.60 €

Table B. 12. Financial model of the reference case from year 1 to 4

			1	2	3	4
Investment			0.00M €	-499.80M €	0.00M €	0.00M €
Sales			0.00M €	37.94M €	151.77M €	154.05M €
Maintenance			0.00M €	-8.29M €	-33.17M €	-34.00M €
Operating labor			0.00M €	-1.28M €	-5.11M €	-5.18M €
Supervision			0.00M €	-0.32M €	-1.28M €	-1.30M €
Plant overheads			0.00M €	-1.04M €	-4.15M €	-4.21M €
Capital charges	Depreciation		0.00M €	-87.46M €	-87.46M €	-87.46M €
	Loan	Principal	0.00M €	-62.44M €	-64.94M €	-67.54M €
		Interests	0.00M €	-29.99M €	-27.49M €	-24.89M €
Environmental costs			0.00M €	-2.21M €	-8.82M €	-8.82M €
Insurance			0.00M €	-1.66M €	-6.63M €	-6.63M €
License fees and royalties			0.00M €	-0.95M €	-3.79M €	-3.85M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	0.00M €	-0.59M €
	Co/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.04M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.07M €
	Fe/Cr/Mg		0.00M €	0.00M €	0.00M €	-0.03M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		0.00M €	-1.56M €	-6.23M €	-6.32M €
	Methanol		0.00M €	-0.07M €	-0.28M €	-0.29M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		0.00M €	-0.05M €	-0.20M €	-0.20M €
Utilities	Water		0.00M €	-0.13M €	-0.52M €	-0.53M €
	Refrigerating water		0.00M €	0.00M €	-0.02M €	-0.02M €
	Softened water		0.00M €	-0.01M €	-0.05M €	-0.05M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		0.00M €	-0.63M €	-2.52M €	-2.57M €
Operating materials			0.00M €	-0.83M €	-3.32M €	-3.40M €
EBITDA			0.00M €	-480.87M €	75.70M €	75.95M €
EBIT			0.00M €	-568.34M €	-11.77M €	-11.52M €
EBT			0.00M €	-598.32M €	-39.26M €	-36.41M €
Taxes			0.00M €	0.00M €	0.00M €	0.00M €
EAT			0.00M €	-598.32M €	-39.26M €	-36.41M €
Cash flow			0.00M €	-573.30M €	-16.74M €	-16.48M €
Cumulative cash flow			0.00M €	-573.30M €	-590.04M €	-606.52M €
Discounted cash flow			0.00M €	-546.00M €	-15.18M €	-14.24M €
Net present value			0.00M €	-546.00M €	-561.18M €	-575.42M €

Table B. 13. Financial model of the reference case from year 5 to 8

			5	6	7	8
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	156.36M €	158.71M €	161.09M €	163.50M €
		Maintenance	-34.85M €	-35.72M €	-36.61M €	-37.53M €
		Operating labor	-5.26M €	-5.34M €	-5.42M €	-5.50M €
		Supervision	-1.32M €	-1.33M €	-1.35M €	-1.38M €
		Plant overheads	-4.27M €	-4.34M €	-4.40M €	-4.47M €
Capital charges		Depreciation	-87.46M €	-87.46M €	-87.46M €	-87.46M €
	Loan	Principal	-70.24M €	-73.05M €	-75.97M €	-79.01M €
		Interests	-22.19M €	-19.38M €	-16.46M €	-13.42M €
		Environmental costs	-8.82M €	-8.82M €	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €	-6.63M €	-6.63M €
		License fees and royalties	-3.91M €	-3.97M €	-4.03M €	-4.09M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.68M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.05M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.08M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.04M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-6.41M €	-6.51M €	-6.61M €	-6.71M €
		Methanol	-0.29M €	-0.30M €	-0.30M €	-0.31M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.21M €	-0.21M €	-0.21M €	-0.22M €
Utilities		Water	-0.54M €	-0.55M €	-0.56M €	-0.58M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.05M €	-0.05M €	-0.05M €	-0.05M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-2.62M €	-2.67M €	-2.72M €	-2.78M €
		Operating materials	-3.49M €	-3.57M €	-3.66M €	-3.75M €
		EBITDA	77.67M €	78.67M €	78.82M €	80.68M €
		EBIT	-9.79M €	-8.79M €	-8.64M €	-6.78M €
		EBT	-31.98M €	-28.17M €	-25.10M €	-20.20M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	-31.98M €	-28.17M €	-25.10M €	-20.20M €
		Cash flow	-14.76M €	-13.76M €	-13.61M €	-11.75M €
		Cumulative cash flow	-621.28M €	-635.04M €	-648.64M €	-660.39M €
		Discounted cash flow	-12.14M €	-10.78M €	-10.15M €	-8.35M €
		Net present value	-587.56M €	-598.34M €	-608.49M €	-616.84M €

Table B. 14. Financial model of the reference case from year 9 to 12

			9	10	11	12
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	165.96M €	168.45M €	170.97M €	173.54M €
		Maintenance	-38.47M €	-39.43M €	-40.42M €	-41.43M €
		Operating labor	-5.58M €	-5.67M €	-5.75M €	-5.84M €
		Supervision	-1.40M €	-1.42M €	-1.44M €	-1.46M €
		Plant overheads	-4.54M €	-4.60M €	-4.67M €	-4.74M €
Capital charges		Depreciation	-87.46M €	-87.46M €	-87.46M €	-87.46M €
	Loan	Principal	-82.17M €	-85.46M €	-88.88M €	0.00M €
		Interests	-10.26M €	-6.97M €	-3.56M €	0.00M €
		Environmental costs	-8.82M €	-8.82M €	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €	-6.63M €	-6.63M €
		License fees and royalties	-4.15M €	-4.21M €	-4.27M €	-4.34M €
Raw materials		Co/Al2O3	0.00M €	-0.79M €	0.00M €	0.00M €
		Co/Mo/Al2O3	0.00M €	-0.06M €	0.00M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	-0.09M €	0.00M €	0.00M €
		Fe/Cr/Mg	0.00M €	-0.04M €	0.00M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	-0.46M €	0.00M €
		Biomass	-6.81M €	-6.91M €	-7.01M €	-7.12M €
		Methanol	-0.31M €	-0.31M €	-0.32M €	-0.32M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.22M €	-0.22M €	-0.23M €	-0.23M €
Utilities		Water	-0.59M €	-0.60M €	-0.61M €	-0.62M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.05M €	-0.05M €	-0.05M €	-0.05M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-2.83M €	-2.89M €	-2.95M €	-3.01M €
		Operating materials	-3.85M €	-3.94M €	-4.04M €	-4.14M €
		EBITDA	81.69M €	81.73M €	83.27M €	84.76M €
		EBIT	-5.77M €	-5.74M €	-4.20M €	-2.71M €
		EBT	-16.03M €	-12.71M €	-7.75M €	-2.71M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	-16.03M €	-12.71M €	-7.75M €	-2.71M €
		Cash flow	-10.74M €	-10.70M €	-9.16M €	84.76M €
		Cumulative cash flow	-671.13M €	-681.83M €	-690.99M €	-606.24M €
		Discounted cash flow	-7.27M €	-6.90M €	-5.62M €	49.56M €
		Net present value	-624.11M €	-631.01M €	-636.64M €	-587.08M €

Table B. 15. Financial model of the reference case from year 13 to 16

			13	14	15	16
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	176.14M €	178.78M €	181.46M €	184.19M €
		Maintenance	-42.46M €	-43.52M €	-44.61M €	-45.73M €
		Operating labor	-5.93M €	-6.01M €	-6.10M €	-6.20M €
		Supervision	-1.48M €	-1.50M €	-1.53M €	-1.55M €
		Plant overheads	-4.81M €	-4.89M €	-4.96M €	-5.03M €
Capital charges		Depreciation	-87.46M €	-87.46M €	-87.46M €	-24.99M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.82M €	-8.82M €	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €	-6.63M €	-6.63M €
		License fees and royalties	-4.40M €	-4.47M €	-4.54M €	-4.60M €
Raw materials		Co/Al2O3	-0.92M €	0.00M €	0.00M €	-1.06M €
		Co/Mo/Al2O3	-0.07M €	0.00M €	0.00M €	-0.08M €
		Ni/Mo/Al2O3	-0.11M €	0.00M €	0.00M €	-0.12M €
		Fe/Cr/Mg	-0.05M €	0.00M €	0.00M €	-0.05M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-7.22M €	-7.33M €	-7.44M €	-7.55M €
		Methanol	-0.33M €	-0.33M €	-0.34M €	-0.34M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.23M €	-0.24M €	-0.24M €	-0.24M €
Utilities		Water	-0.64M €	-0.65M €	-0.66M €	-0.68M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.06M €	-0.06M €	-0.06M €	-0.06M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-3.07M €	-3.13M €	-3.19M €	-3.25M €
		Operating materials	-4.25M €	-4.35M €	-4.46M €	-4.57M €
		EBITDA	84.65M €	86.82M €	87.85M €	87.58M €
		EBIT	-2.82M €	-0.65M €	0.39M €	62.59M €
		EBT	-2.82M €	-0.65M €	0.39M €	62.59M €
		Taxes	0.00M €	0.00M €	-0.12M €	-18.78M €
		EAT	-2.82M €	-0.65M €	0.27M €	43.81M €
		Cash flow	84.65M €	86.82M €	87.74M €	68.80M €
		Cumulative cash flow	-521.59M €	-434.77M €	-347.04M €	-278.24M €
		Discounted cash flow	47.13M €	46.04M €	44.31M €	33.09M €
		Net present value	-539.95M €	-493.90M €	-449.59M €	-416.50M €

Table B. 16. Financial model of the reference case from year 16 to 20

			17	18	19	20
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	186.95M €	189.75M €	192.60M €	195.49M €
		Maintenance	-46.87M €	-48.04M €	-49.24M €	-50.47M €
		Operating labor	-6.29M €	-6.38M €	-6.48M €	-6.58M €
		Supervision	-1.57M €	-1.60M €	-1.62M €	-1.64M €
		Plant overheads	-5.11M €	-5.19M €	-5.26M €	-5.34M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.82M €	-8.82M €	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €	-6.63M €	-6.63M €
		License fees and royalties	-4.67M €	-4.74M €	-4.81M €	-4.89M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-1.23M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.09M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.14M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.06M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-7.67M €	-7.78M €	-7.90M €	-8.02M €
		Methanol	-0.35M €	-0.35M €	-0.36M €	-0.36M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.25M €	-0.25M €	-0.25M €	-0.26M €
Utilities		Water	-0.69M €	-0.70M €	-0.72M €	-0.73M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.06M €	-0.06M €	-0.06M €	-0.06M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-3.32M €	-3.39M €	-3.45M €	-3.52M €
		Operating materials	-4.69M €	-4.80M €	-4.92M €	-5.05M €
		EBITDA	89.94M €	90.98M €	90.50M €	93.08M €
		EBIT	89.94M €	90.98M €	90.50M €	93.08M €
		EBT	89.94M €	90.98M €	90.50M €	93.08M €
		Taxes	-26.98M €	-27.29M €	-27.15M €	-27.92M €
		EAT	62.95M €	63.69M €	63.35M €	65.15M €
		Cash flow	62.95M €	63.69M €	63.35M €	65.15M €
		Cumulative cash flow	-215.28M €	-151.60M €	-88.24M €	-23.09M €
		Discounted cash flow	28.84M €	27.79M €	26.32M €	25.78M €
		Net present value	-387.66M €	-359.87M €	-333.55M €	-307.76M €

Table B. 17. Financial model of the reference case from year 21 to 24

			21	22	23	24
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			198.42M €	201.40M €	204.42M €	207.48M €
Maintenance			-51.74M €	-53.03M €	-54.36M €	-55.71M €
Operating labor			-6.68M €	-6.78M €	-6.88M €	-6.98M €
Supervision			-1.67M €	-1.69M €	-1.72M €	-1.75M €
Plant overheads			-5.42M €	-5.51M €	-5.59M €	-5.67M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.82M €	-8.82M €	-8.82M €	-8.82M €
Insurance			-6.63M €	-6.63M €	-6.63M €	-6.63M €
License fees and royalties			-4.96M €	-5.03M €	-5.11M €	-5.19M €
Raw materials	Co/Al2O3		0.00M €	-1.42M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.11M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.16M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.07M €	0.00M €	0.00M €
	Pt/Re/Al2O3		-0.75M €	0.00M €	0.00M €	0.00M €
	Biomass		-8.14M €	-8.26M €	-8.38M €	-8.51M €
	Methanol		-0.37M €	-0.38M €	-0.38M €	-0.39M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.26M €	-0.27M €	-0.27M €	-0.27M €
Utilities	Water		-0.75M €	-0.76M €	-0.78M €	-0.79M €
	Refrigerating water		-0.02M €	-0.02M €	-0.02M €	-0.02M €
	Softened water		-0.07M €	-0.07M €	-0.07M €	-0.07M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-3.59M €	-3.67M €	-3.74M €	-3.81M €
Operating materials			-5.17M €	-5.30M €	-5.44M €	-5.57M €
EBITDA			93.37M €	93.41M €	96.23M €	97.29M €
EBIT			93.37M €	93.41M €	96.23M €	97.29M €
EBT			93.37M €	93.41M €	96.23M €	97.29M €
Taxes			-28.01M €	-28.02M €	-28.87M €	-29.19M €
EAT			65.36M €	65.39M €	67.36M €	68.10M €
Cash flow			65.36M €	65.39M €	67.36M €	68.10M €
Cumulative cash flow			42.27M €	107.66M €	175.03M €	243.13M €
Discounted cash flow			24.63M €	23.47M €	23.03M €	22.17M €
Net present value			-283.13M €	-259.66M €	-236.63M €	-214.46M €

Table B. 18. Financial model of the reference case from year 25 to 28

			25	26	27	28
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	210.60M €	213.76M €	216.96M €	220.22M €
		Maintenance	-57.11M €	-58.53M €	-60.00M €	-61.50M €
		Operating labor	-7.08M €	-7.19M €	-7.30M €	-7.41M €
		Supervision	-1.77M €	-1.80M €	-1.82M €	-1.85M €
		Plant overheads	-5.76M €	-5.84M €	-5.93M €	-6.02M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.82M €	-8.82M €	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €	-6.63M €	-6.63M €
		License fees and royalties	-5.26M €	-5.34M €	-5.42M €	-5.51M €
Raw materials		Co/Al2O3	-1.65M €	0.00M €	0.00M €	-1.91M €
		Co/Mo/Al2O3	-0.12M €	0.00M €	0.00M €	-0.14M €
		Ni/Mo/Al2O3	-0.19M €	0.00M €	0.00M €	-0.22M €
		Fe/Cr/Mg	-0.08M €	0.00M €	0.00M €	-0.10M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-8.64M €	-8.77M €	-8.90M €	-9.03M €
		Methanol	-0.39M €	-0.40M €	-0.41M €	-0.41M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.28M €	-0.28M €	-0.29M €	-0.29M €
Utilities		Water	-0.81M €	-0.82M €	-0.84M €	-0.86M €
		Refrigerating water	-0.03M €	-0.03M €	-0.03M €	-0.03M €
		Softened water	-0.07M €	-0.07M €	-0.07M €	-0.07M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-3.89M €	-3.97M €	-4.05M €	-4.13M €
		Operating materials	-5.71M €	-5.85M €	-6.00M €	-6.15M €
		EBITDA	96.30M €	99.40M €	100.45M €	99.14M €
		EBIT	96.30M €	99.40M €	100.45M €	99.14M €
		EBT	96.30M €	99.40M €	100.45M €	99.14M €
		Taxes	-28.89M €	-29.82M €	-30.14M €	-29.74M €
		EAT	67.41M €	69.58M €	70.32M €	69.40M €
		Cash flow	67.41M €	69.58M €	70.32M €	69.40M €
		Cumulative cash flow	310.54M €	380.11M €	450.43M €	519.83M €
		Discounted cash flow	20.90M €	20.55M €	19.78M €	18.59M €
		Net present value	-193.56M €	-173.01M €	-153.23M €	-134.65M €

Table B. 19. Financial model of the reference case from year 29 to 30

			29	30
		Investment	0.00M €	0.00M €
		Sales	223.52M €	226.87M €
		Maintenance	-63.04M €	-64.61M €
		Operating labor	-7.52M €	-7.63M €
		Supervision	-1.88M €	-1.91M €
		Plant overheads	-6.11M €	-6.20M €
Capital charges		Depreciation	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €
		Interests	0.00M €	0.00M €
		Environmental costs	-8.82M €	-8.82M €
		Insurance	-6.63M €	-6.63M €
		License fees and royalties	-5.59M €	-5.67M €
Raw materials		Co/Al2O3	0.00M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €
		Biomass	-9.17M €	-9.31M €
		Methanol	-0.42M €	-0.42M €
		Sulfuric acid	0.00M €	0.00M €
		Sodium hydroxide	-0.30M €	-0.30M €
Utilities		Water	-0.87M €	-0.89M €
		Refrigerating water	-0.03M €	-0.03M €
		Softened water	-0.08M €	-0.08M €
		Hydrogen makeup	0.00M €	0.00M €
		Electricity	-4.21M €	-4.29M €
		Operating materials	-6.30M €	-6.46M €
		EBITDA	102.56M €	103.61M €
		EBIT	102.56M €	103.61M €
		EBT	102.56M €	103.61M €
		Taxes	-30.77M €	-31.08M €
		EAT	71.79M €	72.53M €
		Cash flow	71.79M €	72.53M €
		Cumulative cash flow	591.62M €	664.15M €
		Discounted cash flow	18.31M €	17.62M €
		Net present value	-116.33M €	-98.71M €

Table B. 20. CAPEX of the optimal scenario 1

Equipment and Installation	Biomass storage, preparation and feed	17,949,017.53 €
	Biomass air dryer	170,014.25 €
	CFB gasifier, gas cooling and gas cleaning	181,907,154.74 €
	ASU with O2 and N2 compressors	155,985,817.31 €
	Rectisol unit	69,519,813.05 €
	Water gas shift reactor	95,836.61 €
	ATR Reactor	20,392,335.92 €
	PSA	25,085,490.83 €
	Fisher-Tropsch slurry reactor	53,441,270.14 €
	Distillation recovery plant	12,978,203.62 €
	Wax hydrocracker	17,316,400.09 €
	Naphtha hydrotreater	1,612,341.65 €
	Kerosene hydrotreater	4,214,432.47 €
	Diesel hydrotreater	7,570,298.37 €
	Isomerization unit	2,891,672.64 €
	Heavy naphtha reformer	20,186,228.11 €
	Heat recovery steam generator	22,360,618.36 €
	Steam cycle	8,704,601.50 €
	Auxiliary compressors	14,934,746.81 €
	Auxiliary pumps	36,677.71 €
	Co/Al2O3	334,327.19 €
	Co/Mo/Al2O3	23,719.50 €
	Ni/Mo/Al2O3	53,776.98 €
	Fe/Cr/Mg	24,222.72 €
	Pt/Re/Al2O3	177,304.77 €
ISBL		637,966,322.86 €
OSBL		211,208,510.16 €
Engineering and Design		267,736,421.31 €
Contingency		84,856,148.19 €
TOTAL		1,201,767,402.53 €

Table B. 21. Financial model of the optimal scenario 1 from year 1 to 4

			1	2	3	4
Investment			0.00M €	-480.71M €	0.00M €	0.00M €
Sales			0.00M €	40.05M €	160.20M €	162.60M €
Maintenance			0.00M €	-7.97M €	-31.90M €	-32.70M €
Operating labor			0.00M €	-1.28M €	-5.11M €	-5.18M €
Supervision			0.00M €	-0.32M €	-1.28M €	-1.30M €
Plant overheads			0.00M €	-1.04M €	-4.15M €	-4.21M €
Capital charges	Depreciation		0.00M €	-84.12M €	-84.12M €	-84.12M €
	Loan	Principal	0.00M €	-60.06M €	-62.46M €	-64.96M €
		Interests	0.00M €	-28.84M €	-26.44M €	-23.94M €
Environmental costs			0.00M €	-2.12M €	-8.49M €	-8.49M €
Insurance			0.00M €	-1.59M €	-6.38M €	-6.38M €
License fees and royalties			0.00M €	-1.00M €	-4.00M €	-4.06M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	0.00M €	-0.39M €
	Co/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.03M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.06M €
	Fe/Cr/Mg		0.00M €	0.00M €	0.00M €	-0.03M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		0.00M €	-1.56M €	-6.23M €	-6.32M €
	Methanol		0.00M €	-0.08M €	-0.31M €	-0.32M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		0.00M €	-0.05M €	-0.20M €	-0.20M €
Utilities	Water		0.00M €	-0.16M €	-0.63M €	-0.65M €
	Refrigerating water		0.00M €	0.00M €	-0.02M €	-0.02M €
	Softened water		0.00M €	-0.01M €	-0.06M €	-0.06M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		0.00M €	-0.80M €	-3.19M €	-3.27M €
EBITDA			0.00M €	-458.64M €	88.25M €	88.94M €
EBIT			0.00M €	-542.77M €	4.13M €	4.82M €
EBT			0.00M €	-571.61M €	-22.31M €	-19.13M €
Taxes			0.00M €	0.00M €	0.00M €	0.00M €
EAT			0.00M €	-571.61M €	-22.31M €	-19.13M €
Cash flow			0.00M €	-547.54M €	-0.65M €	0.04M €
Cumulative cash flow			0.00M €	-547.54M €	-548.19M €	-548.15M €
Discounted cash flow			0.00M €	-521.47M €	-0.59M €	0.03M €
Net present value			0.00M €	-521.47M €	-522.06M €	-522.02M €

Table B. 22. Financial model of the optimal scenario 1 from year 5 to 8

			5	6	7	8
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	165.04M €	167.51M €	170.03M €	172.58M €
		Maintenance	-33.51M €	-34.35M €	-35.21M €	-36.09M €
		Operating labor	-5.26M €	-5.34M €	-5.42M €	-5.50M €
		Supervision	-1.32M €	-1.33M €	-1.35M €	-1.38M €
		Plant overheads	-4.27M €	-4.34M €	-4.40M €	-4.47M €
Capital charges		Depreciation	-84.12M €	-84.12M €	-84.12M €	-84.12M €
	Loan	Principal	-67.56M €	-70.26M €	-73.07M €	-75.99M €
		Interests	-21.34M €	-18.64M €	-15.83M €	-12.91M €
		Environmental costs	-8.49M €	-8.49M €	-8.49M €	-8.49M €
		Insurance	-6.38M €	-6.38M €	-6.38M €	-6.38M €
		License fees and royalties	-4.13M €	-4.19M €	-4.25M €	-4.31M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.45M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.03M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.07M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.03M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-6.41M €	-6.51M €	-6.61M €	-6.71M €
		Methanol	-0.32M €	-0.33M €	-0.33M €	-0.34M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.21M €	-0.21M €	-0.21M €	-0.22M €
Utilities		Water	-0.66M €	-0.67M €	-0.68M €	-0.70M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.06M €	-0.06M €	-0.06M €	-0.06M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-3.35M €	-3.44M €	-3.52M €	-3.61M €
		EBITDA	90.65M €	91.86M €	92.49M €	94.30M €
		EBIT	6.52M €	7.73M €	8.37M €	10.18M €
		EBT	-14.82M €	-10.91M €	-7.46M €	-2.73M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	-14.82M €	-10.91M €	-7.46M €	-2.73M €
		Cash flow	1.75M €	2.96M €	3.59M €	5.40M €
		Cumulative cash flow	-546.41M €	-543.45M €	-539.86M €	-534.45M €
		Discounted cash flow	1.44M €	2.32M €	2.68M €	3.84M €
		Net present value	-520.59M €	-518.27M €	-515.59M €	-511.75M €

Table B. 23. Financial model of the optimal scenario 1 from year 9 to 12

			9	10	11	12
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			175.17M €	177.79M €	180.46M €	183.17M €
Maintenance			-36.99M €	-37.92M €	-38.87M €	-39.84M €
Operating labor			-5.58M €	-5.67M €	-5.75M €	-5.84M €
Supervision			-1.40M €	-1.42M €	-1.44M €	-1.46M €
Plant overheads			-4.54M €	-4.60M €	-4.67M €	-4.74M €
Capital charges	Depreciation		-84.12M €	-84.12M €	-84.12M €	-84.12M €
	Loan	Principal	-79.03M €	-82.19M €	-85.48M €	0.00M €
		Interests	-9.87M €	-6.71M €	-3.42M €	0.00M €
Environmental costs			-8.49M €	-8.49M €	-8.49M €	-8.49M €
Insurance			-6.38M €	-6.38M €	-6.38M €	-6.38M €
License fees and royalties			-4.38M €	-4.44M €	-4.51M €	-4.58M €
Raw materials	Co/Al2O3		0.00M €	-0.52M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.04M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.08M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.04M €	0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	-0.29M €	0.00M €
	Biomass		-6.81M €	-6.91M €	-7.01M €	-7.12M €
	Methanol		-0.34M €	-0.35M €	-0.35M €	-0.36M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.22M €	-0.22M €	-0.23M €	-0.23M €
Utilities	Water		-0.71M €	-0.73M €	-0.74M €	-0.76M €
	Refrigerating water		-0.02M €	-0.02M €	-0.02M €	-0.02M €
	Softened water		-0.06M €	-0.07M €	-0.07M €	-0.07M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-3.70M €	-3.79M €	-3.89M €	-3.98M €
EBITDA			95.54M €	96.11M €	97.75M €	99.30M €
EBIT			11.42M €	11.99M €	13.63M €	15.18M €
EBT			1.55M €	5.28M €	10.21M €	15.18M €
Taxes			-0.46M €	-1.58M €	-3.06M €	-4.55M €
EAT			1.08M €	3.70M €	7.15M €	10.62M €
Cash flow			6.18M €	5.63M €	5.79M €	94.75M €
Cumulative cash flow			-528.28M €	-522.65M €	-516.86M €	-422.12M €
Discounted cash flow			4.18M €	3.63M €	3.55M €	55.40M €
Net present value			-507.57M €	-503.94M €	-500.39M €	-444.99M €

Table B. 24. Financial model of the optimal scenario 1 from year 13 to 16

			13	14	15	16
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			185.91M €	188.70M €	191.53M €	194.41M €
Maintenance			-40.83M €	-41.85M €	-42.90M €	-43.97M €
Operating labor			-5.93M €	-6.01M €	-6.10M €	-6.20M €
Supervision			-1.48M €	-1.50M €	-1.53M €	-1.55M €
Plant overheads			-4.81M €	-4.89M €	-4.96M €	-5.03M €
Capital charges	Depreciation		-84.12M €	-84.12M €	-84.12M €	-24.04M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.49M €	-8.49M €	-8.49M €	-8.49M €
Insurance			-6.38M €	-6.38M €	-6.38M €	-6.38M €
License fees and royalties			-4.65M €	-4.72M €	-4.79M €	-4.86M €
Raw materials	Co/Al2O3		-0.60M €	0.00M €	0.00M €	-0.70M €
	Co/Mo/Al2O3		-0.04M €	0.00M €	0.00M €	-0.05M €
	Ni/Mo/Al2O3		-0.10M €	0.00M €	0.00M €	-0.11M €
	Fe/Cr/Mg		-0.04M €	0.00M €	0.00M €	-0.05M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.22M €	-7.33M €	-7.44M €	-7.55M €
	Methanol		-0.36M €	-0.37M €	-0.37M €	-0.38M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.23M €	-0.24M €	-0.24M €	-0.24M €
Utilities	Water		-0.77M €	-0.79M €	-0.80M €	-0.82M €
	Refrigerating water		-0.02M €	-0.02M €	-0.03M €	-0.03M €
	Softened water		-0.07M €	-0.07M €	-0.07M €	-0.07M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-4.08M €	-4.19M €	-4.29M €	-4.40M €
EBITDA			99.79M €	101.85M €	103.14M €	103.52M €
EBIT			15.67M €	17.73M €	19.01M €	79.49M €
EBT			15.67M €	17.73M €	19.01M €	79.49M €
Taxes			-4.70M €	-5.32M €	-5.70M €	-23.85M €
EAT			10.97M €	12.41M €	13.31M €	55.64M €
Cash flow			95.09M €	96.53M €	97.43M €	79.68M €
Cumulative cash flow			-327.03M €	-230.49M €	-133.06M €	-53.38M €
Discounted cash flow			52.95M €	51.19M €	49.21M €	38.33M €
Net present value			-392.04M €	-340.85M €	-291.64M €	-253.31M €

Table B. 25. Financial model of the optimal scenario 1 from year 17 to 20

			17	18	19	20
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			197.32M €	200.28M €	203.29M €	206.34M €
Maintenance			-45.07M €	-46.20M €	-47.35M €	-48.54M €
Operating labor			-6.29M €	-6.38M €	-6.48M €	-6.58M €
Supervision			-1.57M €	-1.60M €	-1.62M €	-1.64M €
Plant overheads			-5.11M €	-5.19M €	-5.26M €	-5.34M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.49M €	-8.49M €	-8.49M €	-8.49M €
Insurance			-6.38M €	-6.38M €	-6.38M €	-6.38M €
License fees and royalties			-4.93M €	-5.01M €	-5.08M €	-5.16M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	-0.80M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €	-0.06M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	-0.13M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €	-0.06M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.67M €	-7.78M €	-7.90M €	-8.02M €
	Methanol		-0.39M €	-0.39M €	-0.40M €	-0.40M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.25M €	-0.25M €	-0.25M €	-0.26M €
Utilities	Water		-0.83M €	-0.85M €	-0.87M €	-0.89M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.08M €	-0.08M €	-0.08M €	-0.08M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-4.51M €	-4.62M €	-4.74M €	-4.85M €
EBITDA			105.73M €	107.04M €	107.31M €	109.68M €
EBIT			105.73M €	107.04M €	107.31M €	109.68M €
EBT			105.73M €	107.04M €	107.31M €	109.68M €
Taxes			-31.72M €	-32.11M €	-32.19M €	-32.90M €
EAT			74.01M €	74.93M €	75.11M €	76.77M €
Cash flow			74.01M €	74.93M €	75.11M €	76.77M €
Cumulative cash flow			20.63M €	95.55M €	170.67M €	247.44M €
Discounted cash flow			33.91M €	32.69M €	31.21M €	30.38M €
Net present value			-219.41M €	-186.72M €	-155.51M €	-125.12M €

Table B. 26. Financial model of the optimal scenario 1 from year 20 to 24

			21	22	23	24
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	209.43M €	212.57M €	215.76M €	219.00M €
		Maintenance	-49.75M €	-50.99M €	-52.27M €	-53.58M €
		Operating labor	-6.68M €	-6.78M €	-6.88M €	-6.98M €
		Supervision	-1.67M €	-1.69M €	-1.72M €	-1.75M €
		Plant overheads	-5.42M €	-5.51M €	-5.59M €	-5.67M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.49M €	-8.49M €	-8.49M €	-8.49M €
		Insurance	-6.38M €	-6.38M €	-6.38M €	-6.38M €
		License fees and royalties	-5.24M €	-5.31M €	-5.39M €	-5.47M €
Raw materials		Co/Al2O3	0.00M €	-0.93M €	0.00M €	0.00M €
		Co/Mo/Al2O3	0.00M €	-0.07M €	0.00M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	-0.15M €	0.00M €	0.00M €
		Fe/Cr/Mg	0.00M €	-0.07M €	0.00M €	0.00M €
		Pt/Re/Al2O3	-0.47M €	0.00M €	0.00M €	0.00M €
		Biomass	-8.14M €	-8.26M €	-8.38M €	-8.51M €
		Methanol	-0.41M €	-0.42M €	-0.42M €	-0.43M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.26M €	-0.27M €	-0.27M €	-0.27M €
Utilities		Water	-0.90M €	-0.92M €	-0.94M €	-0.96M €
		Refrigerating water	-0.03M €	-0.03M €	-0.03M €	-0.03M €
		Softened water	-0.08M €	-0.08M €	-0.08M €	-0.09M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-4.98M €	-5.10M €	-5.23M €	-5.36M €
		EBITDA	110.54M €	111.13M €	113.69M €	115.03M €
		EBIT	110.54M €	111.13M €	113.69M €	115.03M €
		EBT	110.54M €	111.13M €	113.69M €	115.03M €
		Taxes	-33.16M €	-33.34M €	-34.11M €	-34.51M €
		EAT	77.38M €	77.79M €	79.58M €	80.52M €
		Cash flow	77.38M €	77.79M €	79.58M €	80.52M €
		Cumulative cash flow	324.82M €	402.61M €	482.19M €	562.71M €
		Discounted cash flow	29.16M €	27.92M €	27.20M €	26.22M €
		Net present value	-95.96M €	-68.04M €	-40.84M €	-14.62M €

Table B. 27. Financial model of the optimal scenario 1 from year 25 to 28

			25	26	27	28
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			222.28M €	225.62M €	229.00M €	232.44M €
Maintenance			-54.92M €	-56.29M €	-57.70M €	-59.14M €
Operating labor			-7.08M €	-7.19M €	-7.30M €	-7.41M €
Supervision			-1.77M €	-1.80M €	-1.82M €	-1.85M €
Plant overheads			-5.76M €	-5.84M €	-5.93M €	-6.02M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.49M €	-8.49M €	-8.49M €	-8.49M €
Insurance			-6.38M €	-6.38M €	-6.38M €	-6.38M €
License fees and royalties			-5.56M €	-5.64M €	-5.73M €	-5.81M €
Raw materials	Co/Al2O3		-1.08M €	0.00M €	0.00M €	-1.25M €
	Co/Mo/Al2O3		-0.08M €	0.00M €	0.00M €	-0.09M €
	Ni/Mo/Al2O3		-0.17M €	0.00M €	0.00M €	-0.20M €
	Fe/Cr/Mg		-0.08M €	0.00M €	0.00M €	-0.09M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-8.64M €	-8.77M €	-8.90M €	-9.03M €
	Methanol		-0.43M €	-0.44M €	-0.45M €	-0.45M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.28M €	-0.28M €	-0.29M €	-0.29M €
Utilities	Water		-0.98M €	-1.00M €	-1.02M €	-1.04M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.09M €	-0.09M €	-0.09M €	-0.09M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-5.49M €	-5.63M €	-5.77M €	-5.91M €
EBITDA			114.98M €	117.75M €	119.11M €	118.85M €
EBIT			114.98M €	117.75M €	119.11M €	118.85M €
EBT			114.98M €	117.75M €	119.11M €	118.85M €
Taxes			-34.49M €	-35.32M €	-35.73M €	-35.66M €
EAT			80.49M €	82.42M €	83.38M €	83.20M €
Cash flow			80.49M €	82.42M €	83.38M €	83.20M €
Cumulative cash flow			643.20M €	725.62M €	809.00M €	892.20M €
Discounted cash flow			24.96M €	24.34M €	23.45M €	22.28M €
Net present value			10.34M €	34.68M €	58.13M €	80.41M €

Table B. 28. Financial model of the optimal scenario 1 from year 29 to 30

			29	30
Investment			0.00M €	0.00M €
Sales			235.92M €	239.46M €
Maintenance			-60.62M €	-62.13M €
Operating labor			-7.52M €	-7.63M €
Supervision			-1.88M €	-1.91M €
Plant overheads			-6.11M €	-6.20M €
Capital charges	Depreciation		0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €
		Interests	0.00M €	0.00M €
Environmental costs			-8.49M €	-8.49M €
Insurance			-6.38M €	-6.38M €
License fees and royalties			-5.90M €	-5.99M €
Raw materials	Co/Al2O3		0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €
	Biomass		-9.17M €	-9.31M €
	Methanol		-0.46M €	-0.47M €
	Sulfuric acid		0.00M €	0.00M €
	Sodium hydroxide		-0.30M €	-0.30M €
Utilities	Water		-1.06M €	-1.08M €
	Refrigerating water		-0.03M €	-0.03M €
	Softened water		-0.10M €	-0.10M €
	Hydrogen makeup		0.00M €	0.00M €
	Electricity		-6.06M €	-6.21M €
EBITDA			121.85M €	123.23M €
EBIT			121.85M €	123.23M €
EBT			121.85M €	123.23M €
Taxes			-36.56M €	-36.97M €
EAT			85.30M €	86.26M €
Cash flow			85.30M €	86.26M €
Cumulative cash flow			977.49M €	1,063.76M €
Discounted cash flow			21.76M €	20.96M €
Net present value			102.17M €	123.13M €

Table B. 29. CAPEX of the optimal scenario 2

Equipment and Installation	Biomass storage, preparation and feed	17,949,017.53 €
	Biomass air dryer	170,014.25 €
	CFB gasifier, gas cooling and gas cleaning	181,907,154.74 €
	ASU with O2 and N2 compressors	170,907,783.90 €
	Rectisol unit	60,965,920.68 €
	Water gas shift reactor	203,941.05 €
	ATR Reactor	15,479,092.51 €
	PSA	22,680,592.87 €
	Fisher-Tropsch slurry reactor	50,304,676.82 €
	Distillation recovery plant	12,315,403.05 €
	Wax hydrocracker	16,634,237.25 €
	Naphtha hydrotreater	1,588,594.95 €
	Kerosene hydrotreater	3,984,254.53 €
	Diesel hydrotreater	7,195,336.39 €
	Isomerization unit	2,851,035.59 €
	Heavy naphtha reformer	19,220,786.10 €
	Heat recovery steam generator	28,382,549.97 €
	Steam cycle	13,752,239.79 €
	Auxiliary compressors	14,378,868.59 €
	Auxiliary pumps	41,393.48 €
	Co/Al2O3	296,227.43 €
	Co/Mo/Al2O3	21,978.96 €
	Ni/Mo/Al2O3	41,375.53 €
	Fe/Cr/Mg	18,636.75 €
	Pt/Re/Al2O3	165,418.99 €
ISBL		641,456,531.74 €
OSBL		212,276,486.87 €
Engineering and Design		269,356,185.99 €
Contingency		85,318,938.09 €
TOTAL		1,208,408,142.69 €

Table B. 30. Financial model of the optimal scenario 2 from year 1 to 4

			1	2	3	4
Investment			0.00M €	-483.36M €	0.00M €	0.00M €
Sales			0.00M €	38.10M €	152.41M €	154.70M €
Maintenance			0.00M €	-8.02M €	-32.07M €	-32.87M €
Operating labor			0.00M €	-1.28M €	-5.11M €	-5.18M €
Supervision			0.00M €	-0.32M €	-1.28M €	-1.30M €
Plant overheads			0.00M €	-1.04M €	-4.15M €	-4.21M €
Capital charges	Depreciation		0.00M €	-84.59M €	-84.59M €	-84.59M €
	Loan	Principal	0.00M €	-60.39M €	-62.81M €	-65.32M €
		Interests	0.00M €	-29.00M €	-26.59M €	-24.07M €
Environmental costs			0.00M €	-2.13M €	-8.54M €	-8.54M €
Insurance			0.00M €	-1.60M €	-6.41M €	-6.41M €
License fees and royalties			0.00M €	-0.95M €	-3.81M €	-3.87M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	0.00M €	-0.34M €
	Co/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.03M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.05M €
	Fe/Cr/Mg		0.00M €	0.00M €	0.00M €	-0.02M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		0.00M €	-1.56M €	-6.23M €	-6.32M €
	Methanol		0.00M €	-0.08M €	-0.32M €	-0.33M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		0.00M €	-0.05M €	-0.20M €	-0.20M €
Utilities	Water		0.00M €	-0.21M €	-0.85M €	-0.86M €
	Refrigerating water		0.00M €	-0.01M €	-0.03M €	-0.03M €
	Softened water		0.00M €	-0.02M €	-0.09M €	-0.09M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		0.00M €	-0.80M €	-3.21M €	-3.29M €
EBITDA			0.00M €	-463.33M €	80.12M €	80.75M €
EBIT			0.00M €	-547.92M €	-4.47M €	-3.83M €
EBT			0.00M €	-576.92M €	-31.05M €	-27.91M €
Taxes			0.00M €	0.00M €	0.00M €	0.00M €
EAT			0.00M €	-576.92M €	-31.05M €	-27.91M €
Cash flow			0.00M €	-552.72M €	-9.27M €	-8.64M €
Cumulative cash flow			0.00M €	-552.72M €	-561.99M €	-570.63M €
Discounted cash flow			0.00M €	-526.40M €	-8.41M €	-7.46M €
Net present value			0.00M €	-526.40M €	-534.81M €	-542.27M €

Table B. 31. Financial model of the optimal scenario 2 from year 5 to 8

			5	6	7	8
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	157.02M €	159.37M €	161.76M €	164.19M €
		Maintenance	-33.70M €	-34.54M €	-35.40M €	-36.29M €
		Operating labor	-5.26M €	-5.34M €	-5.42M €	-5.50M €
		Supervision	-1.32M €	-1.33M €	-1.35M €	-1.38M €
		Plant overheads	-4.27M €	-4.34M €	-4.40M €	-4.47M €
Capital charges		Depreciation	-84.59M €	-84.59M €	-84.59M €	-84.59M €
	Loan	Principal	-67.93M €	-70.65M €	-73.47M €	-76.41M €
		Interests	-21.46M €	-18.74M €	-15.92M €	-12.98M €
		Environmental costs	-8.54M €	-8.54M €	-8.54M €	-8.54M €
		Insurance	-6.41M €	-6.41M €	-6.41M €	-6.41M €
		License fees and royalties	-3.93M €	-3.98M €	-4.04M €	-4.10M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.40M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.03M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.06M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.02M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-6.41M €	-6.51M €	-6.61M €	-6.71M €
		Methanol	-0.33M €	-0.34M €	-0.34M €	-0.35M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.21M €	-0.21M €	-0.21M €	-0.22M €
Utilities		Water	-0.88M €	-0.90M €	-0.92M €	-0.93M €
		Refrigerating water	-0.03M €	-0.03M €	-0.03M €	-0.03M €
		Softened water	-0.09M €	-0.10M €	-0.10M €	-0.10M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-3.37M €	-3.45M €	-3.54M €	-3.63M €
		EBITDA	82.27M €	83.35M €	83.93M €	85.54M €
		EBIT	-2.32M €	-1.24M €	-0.66M €	0.95M €
		EBT	-23.78M €	-19.98M €	-16.57M €	-12.03M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	-23.78M €	-19.98M €	-16.57M €	-12.03M €
		Cash flow	-7.12M €	-6.04M €	-5.46M €	-3.86M €
		Cumulative cash flow	-577.75M €	-583.80M €	-589.25M €	-593.11M €
		Discounted cash flow	-5.86M €	-4.73M €	-4.07M €	-2.74M €
		Net present value	-548.13M €	-552.87M €	-556.94M €	-559.68M €

Table B. 32. Financial model of the optimal scenario 2 from year 9 to 12

			9	10	11	12
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			166.65M €	169.15M €	171.69M €	174.26M €
Maintenance			-37.19M €	-38.12M €	-39.08M €	-40.05M €
Operating labor			-5.58M €	-5.67M €	-5.75M €	-5.84M €
Supervision			-1.40M €	-1.42M €	-1.44M €	-1.46M €
Plant overheads			-4.54M €	-4.60M €	-4.67M €	-4.74M €
Capital charges	Depreciation		-84.59M €	-84.59M €	-84.59M €	-84.59M €
	Loan	Principal	-79.47M €	-82.65M €	-85.95M €	0.00M €
		Interests	-9.92M €	-6.74M €	-3.44M €	0.00M €
Environmental costs			-8.54M €	-8.54M €	-8.54M €	-8.54M €
Insurance			-6.41M €	-6.41M €	-6.41M €	-6.41M €
License fees and royalties			-4.17M €	-4.23M €	-4.29M €	-4.36M €
Raw materials	Co/Al2O3		0.00M €	-0.46M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.03M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.06M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.03M €	0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	-0.27M €	0.00M €
	Biomass		-6.81M €	-6.91M €	-7.01M €	-7.12M €
	Methanol		-0.35M €	-0.36M €	-0.36M €	-0.37M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.22M €	-0.22M €	-0.23M €	-0.23M €
Utilities	Water		-0.95M €	-0.97M €	-0.99M €	-1.01M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.10M €	-0.10M €	-0.11M €	-0.11M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-3.72M €	-3.81M €	-3.91M €	-4.01M €
EBITDA			86.64M €	87.16M €	88.59M €	89.98M €
EBIT			2.05M €	2.57M €	4.01M €	5.40M €
EBT			-7.87M €	-4.17M €	0.57M €	5.40M €
Taxes			0.00M €	0.00M €	-0.17M €	-1.62M €
EAT			-7.87M €	-4.17M €	0.40M €	3.78M €
Cash flow			-2.75M €	-2.23M €	-0.97M €	88.37M €
Cumulative cash flow			-595.86M €	-598.09M €	-599.06M €	-510.70M €
Discounted cash flow			-1.86M €	-1.44M €	-0.59M €	51.67M €
Net present value			-561.54M €	-562.98M €	-563.58M €	-511.91M €

Table B. 33. Financial model of the optimal scenario 2 from year 13 to 16

			13	14	15	16
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			176.88M €	179.53M €	182.22M €	184.96M €
Maintenance			-41.06M €	-42.08M €	-43.13M €	-44.21M €
Operating labor			-5.93M €	-6.01M €	-6.10M €	-6.20M €
Supervision			-1.48M €	-1.50M €	-1.53M €	-1.55M €
Plant overheads			-4.81M €	-4.89M €	-4.96M €	-5.03M €
Capital charges	Depreciation		-84.59M €	-84.59M €	-84.59M €	-24.17M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.54M €	-8.54M €	-8.54M €	-8.54M €
Insurance			-6.41M €	-6.41M €	-6.41M €	-6.41M €
License fees and royalties			-4.42M €	-4.49M €	-4.56M €	-4.62M €
Raw materials	Co/Al2O3		-0.53M €	0.00M €	0.00M €	-0.62M €
	Co/Mo/Al2O3		-0.04M €	0.00M €	0.00M €	-0.05M €
	Ni/Mo/Al2O3		-0.07M €	0.00M €	0.00M €	-0.09M €
	Fe/Cr/Mg		-0.03M €	0.00M €	0.00M €	-0.04M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.22M €	-7.33M €	-7.44M €	-7.55M €
	Methanol		-0.37M €	-0.38M €	-0.38M €	-0.39M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.23M €	-0.24M €	-0.24M €	-0.24M €
Utilities	Water		-1.03M €	-1.05M €	-1.07M €	-1.10M €
	Refrigerating water		-0.04M €	-0.04M €	-0.04M €	-0.04M €
	Softened water		-0.11M €	-0.11M €	-0.11M €	-0.12M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-4.11M €	-4.21M €	-4.31M €	-4.42M €
EBITDA			90.43M €	92.25M €	93.39M €	93.74M €
EBIT			5.84M €	7.66M €	8.80M €	69.58M €
EBT			5.84M €	7.66M €	8.80M €	69.58M €
Taxes			-1.75M €	-2.30M €	-2.64M €	-20.87M €
EAT			4.09M €	5.36M €	6.16M €	48.70M €
Cash flow			88.68M €	89.95M €	90.75M €	72.87M €
Cumulative cash flow			-422.02M €	-332.07M €	-241.32M €	-168.45M €
Discounted cash flow			49.38M €	47.70M €	45.83M €	35.05M €
Net present value			-462.53M €	-414.83M €	-368.99M €	-333.94M €

Table B. 34. Financial model of the optimal scenario 2 from year 17 to 20

			17	18	19	20
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	187.73M €	190.55M €	193.40M €	196.31M €
		Maintenance	-45.32M €	-46.45M €	-47.61M €	-48.80M €
		Operating labor	-6.29M €	-6.38M €	-6.48M €	-6.58M €
		Supervision	-1.57M €	-1.60M €	-1.62M €	-1.64M €
		Plant overheads	-5.11M €	-5.19M €	-5.26M €	-5.34M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.54M €	-8.54M €	-8.54M €	-8.54M €
		Insurance	-6.41M €	-6.41M €	-6.41M €	-6.41M €
		License fees and royalties	-4.69M €	-4.76M €	-4.84M €	-4.91M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.71M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.05M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.10M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.04M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-7.67M €	-7.78M €	-7.90M €	-8.02M €
		Methanol	-0.40M €	-0.40M €	-0.41M €	-0.41M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.25M €	-0.25M €	-0.25M €	-0.26M €
Utilities		Water	-1.12M €	-1.14M €	-1.16M €	-1.19M €
		Refrigerating water	-0.04M €	-0.04M €	-0.04M €	-0.04M €
		Softened water	-0.12M €	-0.12M €	-0.12M €	-0.13M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-4.53M €	-4.65M €	-4.76M €	-4.88M €
		EBITDA	95.68M €	96.83M €	97.08M €	99.16M €
		EBIT	95.68M €	96.83M €	97.08M €	99.16M €
		EBT	95.68M €	96.83M €	97.08M €	99.16M €
		Taxes	-28.70M €	-29.05M €	-29.12M €	-29.75M €
		EAT	66.98M €	67.78M €	67.96M €	69.41M €
		Cash flow	66.98M €	67.78M €	67.96M €	69.41M €
		Cumulative cash flow	-101.47M €	-33.69M €	34.27M €	103.68M €
		Discounted cash flow	30.68M €	29.57M €	28.24M €	27.47M €
		Net present value	-303.26M €	-273.69M €	-245.45M €	-217.98M €

Table B. 35. Financial model of the optimal scenario 2 from year 21 to 24

			21	22	23	24
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	199.25M €	202.24M €	205.27M €	208.35M €
		Maintenance	-50.02M €	-51.27M €	-52.56M €	-53.87M €
		Operating labor	-6.68M €	-6.78M €	-6.88M €	-6.98M €
		Supervision	-1.67M €	-1.69M €	-1.72M €	-1.75M €
		Plant overheads	-5.42M €	-5.51M €	-5.59M €	-5.67M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.54M €	-8.54M €	-8.54M €	-8.54M €
		Insurance	-6.41M €	-6.41M €	-6.41M €	-6.41M €
		License fees and royalties	-4.98M €	-5.06M €	-5.13M €	-5.21M €
Raw materials		Co/Al2O3	0.00M €	-0.83M €	0.00M €	0.00M €
		Co/Mo/Al2O3	0.00M €	-0.06M €	0.00M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	-0.12M €	0.00M €	0.00M €
		Fe/Cr/Mg	0.00M €	-0.05M €	0.00M €	0.00M €
		Pt/Re/Al2O3	-0.44M €	0.00M €	0.00M €	0.00M €
		Biomass	-8.14M €	-8.26M €	-8.38M €	-8.51M €
		Methanol	-0.42M €	-0.43M €	-0.43M €	-0.44M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.26M €	-0.27M €	-0.27M €	-0.27M €
Utilities		Water	-1.21M €	-1.23M €	-1.26M €	-1.28M €
		Refrigerating water	-0.04M €	-0.04M €	-0.04M €	-0.04M €
		Softened water	-0.13M €	-0.13M €	-0.13M €	-0.14M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-5.00M €	-5.13M €	-5.26M €	-5.39M €
		EBITDA	99.89M €	100.44M €	102.67M €	103.85M €
		EBIT	99.89M €	100.44M €	102.67M €	103.85M €
		EBT	99.89M €	100.44M €	102.67M €	103.85M €
		Taxes	-29.97M €	-30.13M €	-30.80M €	-31.16M €
		EAT	69.92M €	70.31M €	71.87M €	72.70M €
		Cash flow	69.92M €	70.31M €	71.87M €	72.70M €
		Cumulative cash flow	173.60M €	243.91M €	315.78M €	388.48M €
		Discounted cash flow	26.35M €	25.24M €	24.57M €	23.67M €
		Net present value	-191.63M €	-166.39M €	-141.82M €	-118.15M €

Table B. 36. Financial model of the optimal scenario 2 from year 25 to 28

			25	26	27	28
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			211.48M €	214.65M €	217.87M €	221.14M €
Maintenance			-55.22M €	-56.60M €	-58.01M €	-59.46M €
Operating labor			-7.08M €	-7.19M €	-7.30M €	-7.41M €
Supervision			-1.77M €	-1.80M €	-1.82M €	-1.85M €
Plant overheads			-5.76M €	-5.84M €	-5.93M €	-6.02M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.54M €	-8.54M €	-8.54M €	-8.54M €
Insurance			-6.41M €	-6.41M €	-6.41M €	-6.41M €
License fees and royalties			-5.29M €	-5.37M €	-5.45M €	-5.53M €
Raw materials	Co/Al2O3		-0.96M €	0.00M €	0.00M €	-1.11M €
	Co/Mo/Al2O3		-0.07M €	0.00M €	0.00M €	-0.08M €
	Ni/Mo/Al2O3		-0.13M €	0.00M €	0.00M €	-0.15M €
	Fe/Cr/Mg		-0.06M €	0.00M €	0.00M €	-0.07M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-8.64M €	-8.77M €	-8.90M €	-9.03M €
	Methanol		-0.45M €	-0.45M €	-0.46M €	-0.47M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.28M €	-0.28M €	-0.29M €	-0.29M €
Utilities	Water		-1.31M €	-1.34M €	-1.36M €	-1.39M €
	Refrigerating water		-0.04M €	-0.05M €	-0.05M €	-0.05M €
	Softened water		-0.14M €	-0.14M €	-0.15M €	-0.15M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-5.52M €	-5.66M €	-5.80M €	-5.95M €
EBITDA			103.81M €	106.22M €	107.41M €	107.18M €
EBIT			103.81M €	106.22M €	107.41M €	107.18M €
EBT			103.81M €	106.22M €	107.41M €	107.18M €
Taxes			-31.14M €	-31.87M €	-32.22M €	-32.16M €
EAT			72.67M €	74.35M €	75.18M €	75.03M €
Cash flow			72.67M €	74.35M €	75.18M €	75.03M €
Cumulative cash flow			461.15M €	535.50M €	610.68M €	685.71M €
Discounted cash flow			22.53M €	21.96M €	21.14M €	20.10M €
Net present value			-95.62M €	-73.66M €	-52.52M €	-32.42M €

Table B. 37. Financial model of the optimal scenario 2 from year 29 to 30

			29	30
Investment			0.00M €	0.00M €
Sales			224.45M €	227.82M €
Maintenance			-60.95M €	-62.47M €
Operating labor			-7.52M €	-7.63M €
Supervision			-1.88M €	-1.91M €
Plant overheads			-6.11M €	-6.20M €
Capital charges	Depreciation		0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €
		Interests	0.00M €	0.00M €
Environmental costs			-8.54M €	-8.54M €
Insurance			-6.41M €	-6.41M €
License fees and royalties			-5.61M €	-5.70M €
Raw materials	Co/Al2O3		0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €
	Biomass		-9.17M €	-9.31M €
	Methanol		-0.47M €	-0.48M €
	Sulfuric acid		0.00M €	0.00M €
	Sodium hydroxide		-0.30M €	-0.30M €
Utilities	Water		-1.42M €	-1.45M €
	Refrigerating water		-0.05M €	-0.05M €
	Softened water		-0.15M €	-0.15M €
	Hydrogen makeup		0.00M €	0.00M €
	Electricity		-6.09M €	-6.25M €
EBITDA			109.79M €	110.98M €
EBIT			109.79M €	110.98M €
EBT			109.79M €	110.98M €
Taxes			-32.94M €	-33.29M €
EAT			76.85M €	77.69M €
Cash flow			76.85M €	77.69M €
Cumulative cash flow			762.56M €	840.25M €
Discounted cash flow			19.60M €	18.87M €
Net present value			-12.82M €	6.05M €

Table B. 38. CAPEX of the optimal scenario 3

Equipment and Installation	Biomass storage, preparation and feed	17,949,017.53 €
	Biomass air dryer	170,014.25 €
	CFB gasifier, gas cooling and gas cleaning	181,907,154.74 €
	ASU with O2 and N2 compressors	154,089,312.42 €
	Rectisol unit	70,038,664.33 €
	Water gas shift reactor	524,790.18 €
	ATR Reactor	19,925,466.43 €
	PSA	21,125,310.90 €
	Fisher-Tropsch slurry reactor	66,831,409.46 €
	Distillation recovery plant	15,753,289.45 €
	Wax hydrocracker	20,979,632.31 €
	Naphtha hydrotreater	2,099,619.00 €
	Kerosene hydrotreater	5,021,815.41 €
	Diesel hydrotreater	9,091,475.26 €
	Isomerization unit	3,719,970.24 €
	Heavy naphtha reformer	23,937,428.32 €
	Heat recovery steam generator	20,960,772.50 €
	Steam cycle	7,576,828.06 €
	Auxiliary compressors	13,739,235.08 €
	Auxiliary pumps	34,819.48 €
	Co/Al2O3	459,474.55 €
	Co/Mo/Al2O3	32,517.47 €
	Ni/Mo/Al2O3	61,670.22 €
	Fe/Cr/Mg	27,778.07 €
	Pt/Re/Al2O3	241,801.49 €
ISBL		656,299,267.15 €
OSBL		216,645,426.26 €
Engineering and Design		275,982,410.72 €
Contingency		87,212,145.16 €
TOTAL		1,236,139,249.29 €

Table B. 39. Financial model of the optimal scenario 3 from year 1 to 4

			1	2	3	4
Investment			0.00M €	-494.46M €	0.00M €	0.00M €
Sales			0.00M €	38.88M €	155.53M €	157.87M €
Maintenance			0.00M €	-8.20M €	-32.81M €	-33.64M €
Operating labor			0.00M €	-1.28M €	-5.11M €	-5.18M €
Supervision			0.00M €	-0.32M €	-1.28M €	-1.30M €
Plant overheads			0.00M €	-1.04M €	-4.15M €	-4.21M €
Capital charges	Depreciation		0.00M €	-86.53M €	-86.53M €	-86.53M €
	Loan	Principal	0.00M €	-61.78M €	-64.25M €	-66.82M €
		Interests	0.00M €	-29.67M €	-27.20M €	-24.63M €
Environmental costs			0.00M €	-2.18M €	-8.73M €	-8.73M €
Insurance			0.00M €	-1.64M €	-6.56M €	-6.56M €
License fees and royalties			0.00M €	-0.97M €	-3.89M €	-3.95M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	0.00M €	-0.53M €
	Co/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.04M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	0.00M €	-0.07M €
	Fe/Cr/Mg		0.00M €	0.00M €	0.00M €	-0.03M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		0.00M €	-1.56M €	-6.23M €	-6.32M €
	Methanol		0.00M €	-0.07M €	-0.29M €	-0.30M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		0.00M €	-0.05M €	-0.20M €	-0.20M €
Utilities	Water		0.00M €	-0.13M €	-0.51M €	-0.52M €
	Refrigerating water		0.00M €	0.00M €	-0.02M €	-0.02M €
	Softened water		0.00M €	-0.01M €	-0.05M €	-0.05M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		0.00M €	-0.13M €	-0.51M €	-0.52M €
Operating materials			0.00M €	-0.82M €	-3.28M €	-3.36M €
EBITDA			0.00M €	-473.98M €	81.91M €	82.33M €
EBIT			0.00M €	-560.51M €	-4.62M €	-4.20M €
EBT			0.00M €	-590.17M €	-31.81M €	-28.82M €
Taxes			0.00M €	0.00M €	0.00M €	0.00M €
EAT			0.00M €	-590.17M €	-31.81M €	-28.82M €
Cash flow			0.00M €	-565.42M €	-9.53M €	-9.11M €
Cumulative cash flow			0.00M €	-565.42M €	-574.95M €	-584.06M €
Discounted cash flow			0.00M €	-538.50M €	-8.64M €	-7.87M €
Net present value			0.00M €	-538.50M €	-547.14M €	-555.01M €

Table B. 40. Financial model of the optimal scenario 3 from year 5 to 8

			5	6	7	8
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	160.24M €	162.64M €	165.08M €	167.55M €
		Maintenance	-34.48M €	-35.34M €	-36.22M €	-37.13M €
		Operating labor	-5.26M €	-5.34M €	-5.42M €	-5.50M €
		Supervision	-1.32M €	-1.33M €	-1.35M €	-1.38M €
		Plant overheads	-4.27M €	-4.34M €	-4.40M €	-4.47M €
Capital charges		Depreciation	-86.53M €	-86.53M €	-86.53M €	-86.53M €
	Loan	Principal	-69.49M €	-72.27M €	-75.16M €	-78.17M €
		Interests	-21.95M €	-19.17M €	-16.28M €	-13.28M €
		Environmental costs	-8.73M €	-8.73M €	-8.73M €	-8.73M €
		Insurance	-6.56M €	-6.56M €	-6.56M €	-6.56M €
		License fees and royalties	-4.01M €	-4.07M €	-4.13M €	-4.19M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.62M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.04M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.08M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.04M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-6.41M €	-6.51M €	-6.61M €	-6.71M €
		Methanol	-0.30M €	-0.31M €	-0.31M €	-0.32M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.21M €	-0.21M €	-0.21M €	-0.22M €
Utilities		Water	-0.53M €	-0.55M €	-0.56M €	-0.57M €
		Refrigerating water	-0.02M €	-0.02M €	-0.02M €	-0.02M €
		Softened water	-0.05M €	-0.05M €	-0.05M €	-0.06M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-0.53M €	-0.54M €	-0.55M €	-0.57M €
		Operating materials	-3.45M €	-3.53M €	-3.62M €	-3.71M €
		EBITDA	84.10M €	85.21M €	85.54M €	87.44M €
		EBIT	-2.43M €	-1.32M €	-0.99M €	0.91M €
		EBT	-24.38M €	-20.49M €	-17.27M €	-12.36M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	-24.38M €	-20.49M €	-17.27M €	-12.36M €
		Cash flow	-7.34M €	-6.23M €	-5.90M €	-4.00M €
		Cumulative cash flow	-591.40M €	-597.63M €	-603.53M €	-607.53M €
		Discounted cash flow	-6.04M €	-4.88M €	-4.40M €	-2.84M €
		Net present value	-561.05M €	-565.93M €	-570.33M €	-573.17M €

Table B. 41. Financial model of the optimal scenario 3 from year 9 to 12

			9	10	11	12
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			170.07M €	172.62M €	175.21M €	177.84M €
Maintenance			-38.06M €	-39.01M €	-39.98M €	-40.98M €
Operating labor			-5.58M €	-5.67M €	-5.75M €	-5.84M €
Supervision			-1.40M €	-1.42M €	-1.44M €	-1.46M €
Plant overheads			-4.54M €	-4.60M €	-4.67M €	-4.74M €
Capital charges	Depreciation		-86.53M €	-86.53M €	-86.53M €	-86.53M €
	Loan	Principal	-81.29M €	-84.54M €	-87.93M €	0.00M €
		Interests	-10.15M €	-6.90M €	-3.52M €	0.00M €
Environmental costs			-8.73M €	-8.73M €	-8.73M €	-8.73M €
Insurance			-6.56M €	-6.56M €	-6.56M €	-6.56M €
License fees and royalties			-4.25M €	-4.32M €	-4.38M €	-4.45M €
Raw materials	Co/Al2O3		0.00M €	-0.71M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.05M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.10M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.04M €	0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	-0.39M €	0.00M €
	Biomass		-6.81M €	-6.91M €	-7.01M €	-7.12M €
	Methanol		-0.32M €	-0.32M €	-0.33M €	-0.33M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.22M €	-0.22M €	-0.23M €	-0.23M €
Utilities	Water		-0.58M €	-0.59M €	-0.60M €	-0.61M €
	Refrigerating water		-0.02M €	-0.02M €	-0.02M €	-0.02M €
	Softened water		-0.06M €	-0.06M €	-0.06M €	-0.06M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-0.58M €	-0.59M €	-0.60M €	-0.61M €
Operating materials			-3.81M €	-3.90M €	-4.00M €	-4.10M €
EBITDA			88.57M €	88.80M €	90.45M €	91.99M €
EBIT			2.04M €	2.27M €	3.92M €	5.46M €
EBT			-8.11M €	-4.63M €	0.40M €	5.46M €
Taxes			0.00M €	0.00M €	-0.12M €	-1.64M €
EAT			-8.11M €	-4.63M €	0.28M €	3.82M €
Cash flow			-2.87M €	-2.64M €	-1.11M €	90.35M €
Cumulative cash flow			-610.40M €	-613.04M €	-614.16M €	-523.81M €
Discounted cash flow			-1.94M €	-1.70M €	-0.68M €	52.83M €
Net present value			-575.12M €	-576.82M €	-577.51M €	-524.68M €

Table B. 42. Financial model of the optimal scenario 3 from year 13 to 16

			13	14	15	16
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			180.50M €	183.21M €	185.96M €	188.75M €
Maintenance			-42.01M €	-43.06M €	-44.13M €	-45.24M €
Operating labor			-5.93M €	-6.01M €	-6.10M €	-6.20M €
Supervision			-1.48M €	-1.50M €	-1.53M €	-1.55M €
Plant overheads			-4.81M €	-4.89M €	-4.96M €	-5.03M €
Capital charges	Depreciation		-86.53M €	-86.53M €	-86.53M €	-24.72M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.73M €	-8.73M €	-8.73M €	-8.73M €
Insurance			-6.56M €	-6.56M €	-6.56M €	-6.56M €
License fees and royalties			-4.51M €	-4.58M €	-4.65M €	-4.72M €
Raw materials	Co/Al2O3		-0.83M €	0.00M €	0.00M €	-0.96M €
	Co/Mo/Al2O3		-0.06M €	0.00M €	0.00M €	-0.07M €
	Ni/Mo/Al2O3		-0.11M €	0.00M €	0.00M €	-0.13M €
	Fe/Cr/Mg		-0.05M €	0.00M €	0.00M €	-0.06M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.22M €	-7.33M €	-7.44M €	-7.55M €
	Methanol		-0.34M €	-0.34M €	-0.35M €	-0.36M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.23M €	-0.24M €	-0.24M €	-0.24M €
Utilities	Water		-0.63M €	-0.64M €	-0.65M €	-0.66M €
	Refrigerating water		-0.02M €	-0.02M €	-0.02M €	-0.02M €
	Softened water		-0.06M €	-0.06M €	-0.06M €	-0.06M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-0.62M €	-0.64M €	-0.65M €	-0.66M €
Operating materials			-4.20M €	-4.31M €	-4.41M €	-4.52M €
EBITDA			92.10M €	94.30M €	95.46M €	95.42M €
EBIT			5.57M €	7.77M €	8.93M €	70.70M €
EBT			5.57M €	7.77M €	8.93M €	70.70M €
Taxes			-1.67M €	-2.33M €	-2.68M €	-21.21M €
EAT			3.90M €	5.44M €	6.25M €	49.49M €
Cash flow			90.43M €	91.97M €	92.78M €	74.21M €
Cumulative cash flow			-433.38M €	-341.42M €	-248.63M €	-174.42M €
Discounted cash flow			50.35M €	48.77M €	46.86M €	35.70M €
Net present value			-474.33M €	-425.56M €	-378.69M €	-343.00M €

Table B. 43. Financial model of the optimal scenario 3 from year 17 to 20

			17	18	19	20
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			191.58M €	194.45M €	197.37M €	200.33M €
Maintenance			-46.37M €	-47.53M €	-48.71M €	-49.93M €
Operating labor			-6.29M €	-6.38M €	-6.48M €	-6.58M €
Supervision			-1.57M €	-1.60M €	-1.62M €	-1.64M €
Plant overheads			-5.11M €	-5.19M €	-5.26M €	-5.34M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.73M €	-8.73M €	-8.73M €	-8.73M €
Insurance			-6.56M €	-6.56M €	-6.56M €	-6.56M €
License fees and royalties			-4.79M €	-4.86M €	-4.93M €	-5.01M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	-1.11M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €	-0.08M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	-0.15M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €	-0.07M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.67M €	-7.78M €	-7.90M €	-8.02M €
	Methanol		-0.36M €	-0.37M €	-0.37M €	-0.38M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.25M €	-0.25M €	-0.25M €	-0.26M €
Utilities	Water		-0.68M €	-0.69M €	-0.71M €	-0.72M €
	Refrigerating water		-0.02M €	-0.02M €	-0.02M €	-0.03M €
	Softened water		-0.07M €	-0.07M €	-0.07M €	-0.07M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-0.68M €	-0.69M €	-0.70M €	-0.72M €
Operating materials			-4.64M €	-4.75M €	-4.87M €	-4.99M €
EBITDA			97.80M €	98.98M €	98.77M €	101.36M €
EBIT			97.80M €	98.98M €	98.77M €	101.36M €
EBT			97.80M €	98.98M €	98.77M €	101.36M €
Taxes			-29.34M €	-29.70M €	-29.63M €	-30.41M €
EAT			68.46M €	69.29M €	69.14M €	70.95M €
Cash flow			68.46M €	69.29M €	69.14M €	70.95M €
Cumulative cash flow			-105.96M €	-36.67M €	32.47M €	103.42M €
Discounted cash flow			31.36M €	30.23M €	28.73M €	28.08M €
Net present value			-311.63M €	-281.40M €	-252.67M €	-224.60M €

Table B. 44. Financial model of the optimal scenario 3 from year 21 to 24

			21	22	23	24
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			203.34M €	206.39M €	209.48M €	212.62M €
Maintenance			-51.18M €	-52.46M €	-53.77M €	-55.12M €
Operating labor			-6.68M €	-6.78M €	-6.88M €	-6.98M €
Supervision			-1.67M €	-1.69M €	-1.72M €	-1.75M €
Plant overheads			-5.42M €	-5.51M €	-5.59M €	-5.67M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.73M €	-8.73M €	-8.73M €	-8.73M €
Insurance			-6.56M €	-6.56M €	-6.56M €	-6.56M €
License fees and royalties			-5.08M €	-5.16M €	-5.24M €	-5.32M €
Raw materials	Co/Al2O3		0.00M €	-1.28M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.09M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.17M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.08M €	0.00M €	0.00M €
	Pt/Re/Al2O3		-0.64M €	0.00M €	0.00M €	0.00M €
	Biomass		-8.14M €	-8.26M €	-8.38M €	-8.51M €
	Methanol		-0.38M €	-0.39M €	-0.39M €	-0.40M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.26M €	-0.27M €	-0.27M €	-0.27M €
Utilities	Water		-0.73M €	-0.75M €	-0.76M €	-0.78M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.07M €	-0.07M €	-0.07M €	-0.08M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-0.73M €	-0.75M €	-0.76M €	-0.78M €
Operating materials			-5.12M €	-5.25M €	-5.38M €	-5.51M €
EBITDA			101.91M €	102.13M €	104.95M €	106.15M €
EBIT			101.91M €	102.13M €	104.95M €	106.15M €
EBT			101.91M €	102.13M €	104.95M €	106.15M €
Taxes			-30.57M €	-30.64M €	-31.48M €	-31.85M €
EAT			71.34M €	71.49M €	73.46M €	74.31M €
Cash flow			71.34M €	71.49M €	73.46M €	74.31M €
Cumulative cash flow			174.75M €	246.24M €	319.70M €	394.01M €
Discounted cash flow			26.89M €	25.66M €	25.11M €	24.19M €
Net present value			-197.71M €	-172.05M €	-146.94M €	-122.75M €

Table B. 45. Financial model of the optimal scenario 3 from year 25 to 28

			25	26	27	28
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	215.81M €	219.05M €	222.34M €	225.67M €
		Maintenance	-56.49M €	-57.91M €	-59.35M €	-60.84M €
		Operating labor	-7.08M €	-7.19M €	-7.30M €	-7.41M €
		Supervision	-1.77M €	-1.80M €	-1.82M €	-1.85M €
		Plant overheads	-5.76M €	-5.84M €	-5.93M €	-6.02M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.73M €	-8.73M €	-8.73M €	-8.73M €
		Insurance	-6.56M €	-6.56M €	-6.56M €	-6.56M €
		License fees and royalties	-5.40M €	-5.48M €	-5.56M €	-5.64M €
Raw materials		Co/Al2O3	-1.48M €	0.00M €	0.00M €	-1.72M €
		Co/Mo/Al2O3	-0.10M €	0.00M €	0.00M €	-0.12M €
		Ni/Mo/Al2O3	-0.20M €	0.00M €	0.00M €	-0.23M €
		Fe/Cr/Mg	-0.09M €	0.00M €	0.00M €	-0.10M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-8.64M €	-8.77M €	-8.90M €	-9.03M €
		Methanol	-0.41M €	-0.41M €	-0.42M €	-0.42M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.28M €	-0.28M €	-0.29M €	-0.29M €
Utilities		Water	-0.79M €	-0.81M €	-0.83M €	-0.84M €
		Refrigerating water	-0.03M €	-0.03M €	-0.03M €	-0.03M €
		Softened water	-0.08M €	-0.08M €	-0.08M €	-0.08M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-0.79M €	-0.81M €	-0.82M €	-0.84M €
		Operating materials	-5.65M €	-5.79M €	-5.94M €	-6.08M €
		EBITDA	105.48M €	108.57M €	109.78M €	108.82M €
		EBIT	105.48M €	108.57M €	109.78M €	108.82M €
		EBT	105.48M €	108.57M €	109.78M €	108.82M €
		Taxes	-31.64M €	-32.57M €	-32.93M €	-32.65M €
		EAT	73.84M €	76.00M €	76.85M €	76.18M €
		Cash flow	73.84M €	76.00M €	76.85M €	76.18M €
		Cumulative cash flow	467.85M €	543.84M €	620.69M €	696.86M €
		Discounted cash flow	22.89M €	22.44M €	21.61M €	20.40M €
		Net present value	-99.85M €	-77.41M €	-55.80M €	-35.39M €

Table B. 46. Financial model of the optimal scenario 3 from year 29 to 30

			29	30
Investment			0.00M €	0.00M €
Sales			229.06M €	232.49M €
Maintenance			-62.36M €	-63.92M €
Operating labor			-7.52M €	-7.63M €
Supervision			-1.88M €	-1.91M €
Plant overheads			-6.11M €	-6.20M €
Capital charges	Depreciation		0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €
		Interests	0.00M €	0.00M €
Environmental costs			-8.73M €	-8.73M €
Insurance			-6.56M €	-6.56M €
License fees and royalties			-5.73M €	-5.81M €
Raw materials	Co/Al2O3		0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €
	Biomass		-9.17M €	-9.31M €
	Methanol		-0.43M €	-0.44M €
	Sulfuric acid		0.00M €	0.00M €
	Sodium hydroxide		-0.30M €	-0.30M €
Utilities	Water		-0.86M €	-0.88M €
	Refrigerating water		-0.03M €	-0.03M €
	Softened water		-0.08M €	-0.09M €
	Hydrogen makeup		0.00M €	0.00M €
	Electricity		-0.86M €	-0.87M €
Operating materials			-6.24M €	-6.39M €
EBITDA			112.21M €	113.43M €
EBIT			112.21M €	113.43M €
EBT			112.21M €	113.43M €
Taxes			-33.66M €	-34.03M €
EAT			78.55M €	79.40M €
Cash flow			78.55M €	79.40M €
Cumulative cash flow			775.41M €	854.81M €
Discounted cash flow			20.04M €	19.29M €
Net present value			-15.36M €	3.93M €

Table B. 47. CAPEX of the optimal scenario 4

Equipment and Installation	Biomass storage, preparation and feed	17,949,017.53 €
	Biomass air dryer	170,014.25 €
	CFB gasifier, gas cooling and gas cleaning	181,907,154.74 €
	ASU with O2 and N2 compressors	165,774,915.82 €
	Rectisol unit	62,653,474.34 €
	Water gas shift reactor	128,662.53 €
	ATR Reactor	15,593,798.72 €
	PSA	22,893,222.50 €
	Fisher-Tropsch slurry reactor	54,440,054.58 €
	Distillation recovery plant	13,188,157.55 €
	Wax hydrocracker	17,691,346.23 €
	Naphtha hydrotreater	1,728,592.63 €
	Kerosene hydrotreater	4,243,219.03 €
	Diesel hydrotreater	7,663,792.01 €
	Isomerization unit	3,090,218.72 €
	Heavy naphtha reformer	20,450,031.10 €
	Heat recovery steam generator	26,176,503.45 €
	Steam cycle	11,998,056.23 €
	Auxiliary compressors	14,354,495.99 €
	Auxiliary pumps	40,009.06 €
	Co/Al2O3	324,559.72 €
	Co/Mo/Al2O3	24,496.12 €
	Ni/Mo/Al2O3	43,984.18 €
	Fe/Cr/Mg	19,811.76 €
	Pt/Re/Al2O3	184,480.61 €
ISBL		642,732,069.41 €
OSBL		212,643,039.76 €
Engineering and Design		269,912,124.53 €
Contingency		85,477,777.68 €
TOTAL		1,210,765,011.39 €

Table B. 48. Financial model of the optimal scenario 4 from year 1 to 4

			1	2	3	4
		Investment	0.00M €	-484.31M €	0.00M €	0.00M €
		Sales	0.00M €	38.96M €	155.82M €	158.16M €
		Maintenance	0.00M €	-8.03M €	-32.14M €	-32.94M €
		Operating labor	0.00M €	-1.28M €	-5.11M €	-5.18M €
		Supervision	0.00M €	-0.32M €	-1.28M €	-1.30M €
		Plant overheads	0.00M €	-1.04M €	-4.15M €	-4.21M €
Capital charges		Depreciation	0.00M €	-84.75M €	-84.75M €	-84.75M €
	Loan	Principal	0.00M €	-60.51M €	-62.93M €	-65.44M €
		Interests	0.00M €	-29.06M €	-26.64M €	-24.12M €
		Environmental costs	0.00M €	-2.14M €	-8.55M €	-8.55M €
		Insurance	0.00M €	-1.61M €	-6.43M €	-6.43M €
		License fees and royalties	0.00M €	-0.97M €	-3.90M €	-3.95M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	0.00M €	-0.38M €
		Co/Mo/Al2O3	0.00M €	0.00M €	0.00M €	-0.03M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	0.00M €	-0.05M €
		Fe/Cr/Mg	0.00M €	0.00M €	0.00M €	-0.02M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	0.00M €	-1.56M €	-6.23M €	-6.32M €
		Methanol	0.00M €	-0.08M €	-0.31M €	-0.32M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	0.00M €	-0.05M €	-0.20M €	-0.20M €
Utilities		Water	0.00M €	-0.19M €	-0.77M €	-0.79M €
		Refrigerating water	0.00M €	-0.01M €	-0.03M €	-0.03M €
		Softened water	0.00M €	-0.02M €	-0.08M €	-0.08M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	0.00M €	-0.80M €	-3.21M €	-3.29M €
		EBITDA	0.00M €	-463.45M €	83.44M €	84.08M €
		EBIT	0.00M €	-548.20M €	-1.31M €	-0.67M €
		EBT	0.00M €	-577.26M €	-27.95M €	-24.79M €
		Taxes	0.00M €	0.00M €	0.00M €	0.00M €
		EAT	0.00M €	-577.26M €	-27.95M €	-24.79M €
		Cash flow	0.00M €	-553.01M €	-6.12M €	-5.48M €
		Cumulative cash flow	0.00M €	-553.01M €	-559.13M €	-564.62M €
		Discounted cash flow	0.00M €	-526.68M €	-5.55M €	-4.74M €
		Net present value	0.00M €	-526.68M €	-532.23M €	-536.97M €

Table B. 49. Financial model of the optimal scenario 4 from year 5 to 8

			5	6	7	8
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			160.53M €	162.94M €	165.38M €	167.86M €
Maintenance			-33.76M €	-34.61M €	-35.47M €	-36.36M €
Operating labor			-5.26M €	-5.34M €	-5.42M €	-5.50M €
Supervision			-1.32M €	-1.33M €	-1.35M €	-1.38M €
Plant overheads			-4.27M €	-4.34M €	-4.40M €	-4.47M €
Capital charges	Depreciation		-84.75M €	-84.75M €	-84.75M €	-84.75M €
	Loan	Principal	-68.06M €	-70.79M €	-73.62M €	-76.56M €
		Interests	-21.50M €	-18.78M €	-15.95M €	-13.00M €
Environmental costs			-8.55M €	-8.55M €	-8.55M €	-8.55M €
Insurance			-6.43M €	-6.43M €	-6.43M €	-6.43M €
License fees and royalties			-4.01M €	-4.07M €	-4.13M €	-4.20M €
Raw materials	Co/Al2O3		0.00M €	0.00M €	-0.43M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €	-0.03M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €	-0.06M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €	-0.03M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-6.41M €	-6.51M €	-6.61M €	-6.71M €
	Methanol		-0.32M €	-0.33M €	-0.33M €	-0.34M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.21M €	-0.21M €	-0.21M €	-0.22M €
Utilities	Water		-0.81M €	-0.82M €	-0.84M €	-0.86M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.08M €	-0.08M €	-0.09M €	-0.09M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-3.38M €	-3.46M €	-3.55M €	-3.64M €
EBITDA			85.69M €	86.82M €	87.41M €	89.11M €
EBIT			0.93M €	2.07M €	2.66M €	4.36M €
EBT			-20.57M €	-16.71M €	-13.29M €	-8.64M €
Taxes			0.00M €	0.00M €	0.00M €	0.00M €
EAT			-20.57M €	-16.71M €	-13.29M €	-8.64M €
Cash flow			-3.88M €	-2.74M €	-2.16M €	-0.45M €
Cumulative cash flow			-568.49M €	-571.24M €	-573.39M €	-573.84M €
Discounted cash flow			-3.19M €	-2.15M €	-1.61M €	-0.32M €
Net present value			-540.16M €	-542.31M €	-543.91M €	-544.24M €

Table B. 50. Financial model of the optimal scenario 4 from year 9 to 12

			9	10	11	12
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			170.38M €	172.94M €	175.53M €	178.16M €
Maintenance			-37.27M €	-38.20M €	-39.16M €	-40.13M €
Operating labor			-5.58M €	-5.67M €	-5.75M €	-5.84M €
Supervision			-1.40M €	-1.42M €	-1.44M €	-1.46M €
Plant overheads			-4.54M €	-4.60M €	-4.67M €	-4.74M €
Capital charges	Depreciation		-84.75M €	-84.75M €	-84.75M €	-84.75M €
	Loan	Principal	-79.62M €	-82.81M €	-86.12M €	0.00M €
		Interests	-9.94M €	-6.76M €	-3.44M €	0.00M €
Environmental costs			-8.55M €	-8.55M €	-8.55M €	-8.55M €
Insurance			-6.43M €	-6.43M €	-6.43M €	-6.43M €
License fees and royalties			-4.26M €	-4.32M €	-4.39M €	-4.45M €
Raw materials	Co/Al2O3		0.00M €	-0.50M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.04M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.07M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.03M €	0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €	-0.30M €	0.00M €
	Biomass		-6.81M €	-6.91M €	-7.01M €	-7.12M €
	Methanol		-0.34M €	-0.35M €	-0.35M €	-0.36M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.22M €	-0.22M €	-0.23M €	-0.23M €
Utilities	Water		-0.87M €	-0.89M €	-0.91M €	-0.93M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.09M €	-0.09M €	-0.09M €	-0.09M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-3.73M €	-3.82M €	-3.92M €	-4.01M €
EBITDA			90.27M €	90.79M €	92.30M €	93.78M €
EBIT			5.52M €	6.04M €	7.55M €	9.03M €
EBT			-4.43M €	-0.72M €	4.11M €	9.03M €
Taxes			0.00M €	0.00M €	-1.23M €	-2.71M €
EAT			-4.43M €	-0.72M €	2.87M €	6.32M €
Cash flow			0.70M €	1.23M €	1.51M €	91.07M €
Cumulative cash flow			-573.14M €	-571.91M €	-570.41M €	-479.33M €
Discounted cash flow			0.48M €	0.79M €	0.92M €	53.25M €
Net present value			-543.76M €	-542.97M €	-542.04M €	-488.79M €

Table B. 51. Financial model of the optimal scenario 4 from year 13 to 16

			13	14	15	16
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			180.84M €	183.55M €	186.30M €	189.10M €
Maintenance			-41.14M €	-42.17M €	-43.22M €	-44.30M €
Operating labor			-5.93M €	-6.01M €	-6.10M €	-6.20M €
Supervision			-1.48M €	-1.50M €	-1.53M €	-1.55M €
Plant overheads			-4.81M €	-4.89M €	-4.96M €	-5.03M €
Capital charges	Depreciation		-84.75M €	-84.75M €	-84.75M €	-24.22M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.55M €	-8.55M €	-8.55M €	-8.55M €
Insurance			-6.43M €	-6.43M €	-6.43M €	-6.43M €
License fees and royalties			-4.52M €	-4.59M €	-4.66M €	-4.73M €
Raw materials	Co/Al2O3		-0.58M €	0.00M €	0.00M €	-0.67M €
	Co/Mo/Al2O3		-0.04M €	0.00M €	0.00M €	-0.05M €
	Ni/Mo/Al2O3		-0.08M €	0.00M €	0.00M €	-0.09M €
	Fe/Cr/Mg		-0.04M €	0.00M €	0.00M €	-0.04M €
	Pt/Re/Al2O3		0.00M €	0.00M €	0.00M €	0.00M €
	Biomass		-7.22M €	-7.33M €	-7.44M €	-7.55M €
	Methanol		-0.37M €	-0.37M €	-0.38M €	-0.38M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.23M €	-0.24M €	-0.24M €	-0.24M €
Utilities	Water		-0.94M €	-0.96M €	-0.98M €	-1.00M €
	Refrigerating water		-0.03M €	-0.03M €	-0.03M €	-0.03M €
	Softened water		-0.10M €	-0.10M €	-0.10M €	-0.10M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-4.11M €	-4.22M €	-4.32M €	-4.43M €
EBITDA			94.23M €	96.16M €	97.36M €	97.70M €
EBIT			9.47M €	11.41M €	12.60M €	73.49M €
EBT			9.47M €	11.41M €	12.60M €	73.49M €
Taxes			-2.84M €	-3.42M €	-3.78M €	-22.05M €
EAT			6.63M €	7.98M €	8.82M €	51.44M €
Cash flow			91.38M €	92.74M €	93.58M €	75.66M €
Cumulative cash flow			-387.95M €	-295.21M €	-201.64M €	-125.98M €
Discounted cash flow			50.89M €	49.18M €	47.26M €	36.39M €
Net present value			-437.91M €	-388.73M €	-341.47M €	-305.07M €

Table B. 52. Financial model of the optimal scenario 4 from year 17 to 20

			17	18	19	20
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	191.93M €	194.81M €	197.73M €	200.70M €
		Maintenance	-45.41M €	-46.54M €	-47.71M €	-48.90M €
		Operating labor	-6.29M €	-6.38M €	-6.48M €	-6.58M €
		Supervision	-1.57M €	-1.60M €	-1.62M €	-1.64M €
		Plant overheads	-5.11M €	-5.19M €	-5.26M €	-5.34M €
Capital charges		Depreciation	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.55M €	-8.55M €	-8.55M €	-8.55M €
		Insurance	-6.43M €	-6.43M €	-6.43M €	-6.43M €
		License fees and royalties	-4.80M €	-4.87M €	-4.94M €	-5.02M €
Raw materials		Co/Al2O3	0.00M €	0.00M €	-0.78M €	0.00M €
		Co/Mo/Al2O3	0.00M €	0.00M €	-0.06M €	0.00M €
		Ni/Mo/Al2O3	0.00M €	0.00M €	-0.11M €	0.00M €
		Fe/Cr/Mg	0.00M €	0.00M €	-0.05M €	0.00M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-7.67M €	-7.78M €	-7.90M €	-8.02M €
		Methanol	-0.39M €	-0.39M €	-0.40M €	-0.41M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.25M €	-0.25M €	-0.25M €	-0.26M €
Utilities		Water	-1.02M €	-1.04M €	-1.06M €	-1.08M €
		Refrigerating water	-0.03M €	-0.03M €	-0.04M €	-0.04M €
		Softened water	-0.10M €	-0.11M €	-0.11M €	-0.11M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-4.54M €	-4.65M €	-4.77M €	-4.89M €
		EBITDA	99.77M €	100.99M €	101.21M €	103.44M €
		EBIT	99.77M €	100.99M €	101.21M €	103.44M €
		EBT	99.77M €	100.99M €	101.21M €	103.44M €
		Taxes	-29.93M €	-30.30M €	-30.36M €	-31.03M €
		EAT	69.84M €	70.69M €	70.85M €	72.40M €
		Cash flow	69.84M €	70.69M €	70.85M €	72.40M €
		Cumulative cash flow	-56.14M €	14.55M €	85.40M €	157.81M €
		Discounted cash flow	31.99M €	30.84M €	29.44M €	28.65M €
		Net present value	-273.08M €	-242.24M €	-212.80M €	-184.14M €

Table B. 53. Financial model of the optimal scenario 4 from year 21 to 24

			21	22	23	24
Investment			0.00M €	0.00M €	0.00M €	0.00M €
Sales			203.71M €	206.77M €	209.87M €	213.02M €
Maintenance			-50.12M €	-51.38M €	-52.66M €	-53.98M €
Operating labor			-6.68M €	-6.78M €	-6.88M €	-6.98M €
Supervision			-1.67M €	-1.69M €	-1.72M €	-1.75M €
Plant overheads			-5.42M €	-5.51M €	-5.59M €	-5.67M €
Capital charges	Depreciation		0.00M €	0.00M €	0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
Environmental costs			-8.55M €	-8.55M €	-8.55M €	-8.55M €
Insurance			-6.43M €	-6.43M €	-6.43M €	-6.43M €
License fees and royalties			-5.09M €	-5.17M €	-5.25M €	-5.33M €
Raw materials	Co/Al2O3		0.00M €	-0.90M €	0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	-0.07M €	0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	-0.12M €	0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	-0.06M €	0.00M €	0.00M €
	Pt/Re/Al2O3		-0.49M €	0.00M €	0.00M €	0.00M €
	Biomass		-8.14M €	-8.26M €	-8.38M €	-8.51M €
	Methanol		-0.41M €	-0.42M €	-0.42M €	-0.43M €
	Sulfuric acid		0.00M €	0.00M €	0.00M €	0.00M €
	Sodium hydroxide		-0.26M €	-0.27M €	-0.27M €	-0.27M €
Utilities	Water		-1.11M €	-1.13M €	-1.15M €	-1.17M €
	Refrigerating water		-0.04M €	-0.04M €	-0.04M €	-0.04M €
	Softened water		-0.11M €	-0.11M €	-0.12M €	-0.12M €
	Hydrogen makeup		0.00M €	0.00M €	0.00M €	0.00M €
	Electricity		-5.01M €	-5.14M €	-5.27M €	-5.40M €
EBITDA			104.18M €	104.75M €	107.15M €	108.39M €
EBIT			104.18M €	104.75M €	107.15M €	108.39M €
EBT			104.18M €	104.75M €	107.15M €	108.39M €
Taxes			-31.25M €	-31.43M €	-32.14M €	-32.52M €
EAT			72.92M €	73.33M €	75.00M €	75.87M €
Cash flow			72.92M €	73.33M €	75.00M €	75.87M €
Cumulative cash flow			230.73M €	304.06M €	379.06M €	454.94M €
Discounted cash flow			27.48M €	26.32M €	25.64M €	24.70M €
Net present value			-156.66M €	-130.34M €	-104.70M €	-80.00M €

Table B. 54. Financial model of the optimal scenario 4 from year 25 to 28

			25	26	27	28
		Investment	0.00M €	0.00M €	0.00M €	0.00M €
		Sales	216.21M €	219.45M €	222.75M €	226.09M €
		Maintenance	-55.33M €	-56.71M €	-58.13M €	-59.58M €
		Operating labor	-7.08M €	-7.19M €	-7.30M €	-7.41M €
		Supervision	-1.77M €	-1.80M €	-1.82M €	-1.85M €
		Plant overheads	-5.76M €	-5.84M €	-5.93M €	-6.02M €
Capital charges		**Depreciation**	0.00M €	0.00M €	0.00M €	0.00M €
	Loan	**Principal**	0.00M €	0.00M €	0.00M €	0.00M €
		Interests	0.00M €	0.00M €	0.00M €	0.00M €
		Environmental costs	-8.55M €	-8.55M €	-8.55M €	-8.55M €
		Insurance	-6.43M €	-6.43M €	-6.43M €	-6.43M €
		License fees and royalties	-5.41M €	-5.49M €	-5.57M €	-5.65M €
Raw materials		**Co/Al2O3**	-1.05M €	0.00M €	0.00M €	-1.21M €
		Co/Mo/Al2O3	-0.08M €	0.00M €	0.00M €	-0.09M €
		Ni/Mo/Al2O3	-0.14M €	0.00M €	0.00M €	-0.16M €
		Fe/Cr/Mg	-0.06M €	0.00M €	0.00M €	-0.07M €
		Pt/Re/Al2O3	0.00M €	0.00M €	0.00M €	0.00M €
		Biomass	-8.64M €	-8.77M €	-8.90M €	-9.03M €
		Methanol	-0.44M €	-0.44M €	-0.45M €	-0.46M €
		Sulfuric acid	0.00M €	0.00M €	0.00M €	0.00M €
		Sodium hydroxide	-0.28M €	-0.28M €	-0.29M €	-0.29M €
Utilities		**Water**	-1.20M €	-1.22M €	-1.25M €	-1.27M €
		Refrigerating water	-0.04M €	-0.04M €	-0.04M €	-0.04M €
		Softened water	-0.12M €	-0.12M €	-0.13M €	-0.13M €
		Hydrogen makeup	0.00M €	0.00M €	0.00M €	0.00M €
		Electricity	-5.53M €	-5.67M €	-5.81M €	-5.96M €
		EBITDA	108.31M €	110.90M €	112.15M €	111.87M €
		EBIT	108.31M €	110.90M €	112.15M €	111.87M €
		EBT	108.31M €	110.90M €	112.15M €	111.87M €
		Taxes	-32.49M €	-33.27M €	-33.65M €	-33.56M €
		EAT	75.82M €	77.63M €	78.51M €	78.31M €
		Cash flow	75.82M €	77.63M €	78.51M €	78.31M €
		Cumulative cash flow	530.75M €	608.38M €	686.89M €	765.20M €
		Discounted cash flow	23.51M €	22.92M €	22.08M €	20.98M €
		Net present value	-56.49M €	-33.56M €	-11.48M €	9.49M €

Table B. 55. Financial model of the optimal scenario 4 from year 29 to 30

			29	30
Investment			0.00M €	0.00M €
Sales			229.48M €	232.92M €
Maintenance			-61.07M €	-62.60M €
Operating labor			-7.52M €	-7.63M €
Supervision			-1.88M €	-1.91M €
Plant overheads			-6.11M €	-6.20M €
Capital charges	Depreciation		0.00M €	0.00M €
	Loan	Principal	0.00M €	0.00M €
		Interests	0.00M €	0.00M €
Environmental costs			-8.55M €	-8.55M €
Insurance			-6.43M €	-6.43M €
License fees and royalties			-5.74M €	-5.82M €
Raw materials	Co/Al2O3		0.00M €	0.00M €
	Co/Mo/Al2O3		0.00M €	0.00M €
	Ni/Mo/Al2O3		0.00M €	0.00M €
	Fe/Cr/Mg		0.00M €	0.00M €
	Pt/Re/Al2O3		0.00M €	0.00M €
	Biomass		-9.17M €	-9.31M €
	Methanol		-0.46M €	-0.47M €
	Sulfuric acid		0.00M €	0.00M €
	Sodium hydroxide		-0.30M €	-0.30M €
Utilities	Water		-1.30M €	-1.32M €
	Refrigerating water		-0.04M €	-0.04M €
	Softened water		-0.13M €	-0.13M €
	Hydrogen makeup		0.00M €	0.00M €
	Electricity		-6.11M €	-6.26M €
EBITDA			114.68M €	115.94M €
EBIT			114.68M €	115.94M €
EBT			114.68M €	115.94M €
Taxes			-34.40M €	-34.78M €
EAT			80.27M €	81.16M €
Cash flow			80.27M €	81.16M €
Cumulative cash flow			845.48M €	926.64M €
Discounted cash flow			20.48M €	19.72M €
Net present value			29.97M €	49.69M €

References

Aasberg-Petersen, Kim, Thomas S. Christensen, Charlotte Stub Nielsen, and Ib Dybkjær. 2003. “Recent Developments in Autothermal Reforming and Pre-Reforming for Synthesis Gas Production in GTL Applications.” *Fuel Processing Technology*, Advances in C1 Chemistry in the Year 2002, 83 (1): 253–61. https://doi.org/10.1016/S0378-3820(03)00073-0.

Acciarini, Giacomo, Dario Izzo, and Erwin Mooij. 2020. “MHACO: A Multi-Objective Hypervolume-Based Ant Colony Optimizer for Space Trajectory Optimization.” In *2020 IEEE Congress on Evolutionary Computation (CEC)*, 1–8. https://doi.org/10.1109/CEC48606.2020.9185694.

Ahmadi, Aras, and Ligia Tiruta-Barna. 2015. “A Process Modelling-Life Cycle Assessment-MultiObjective Optimization Tool for the Eco-Design of Conventional Treatment Processes of Potable Water.” *Journal of Cleaner Production* 100 (August): 116–25. https://doi.org/10.1016/j.jclepro.2015.03.045.

Andrews, Evan, Leif-Patrick Barthel, Catherine Norris, Andreas Ciroth, Carmela Cucuzzella, Carl-Otto Gensch, Julie Hebert, et al. 2009. *Guidelines for Social Life Cycle Assessment of Products*.

ASME. 2017. *BPVC Section VIII-Rules for Construction of Pressure Vessels Division 1*. https://www.asme.org/codes-standards/find-codes-standards/bpvc-viii-1-bpvc-section-viii-rules-construction-pressure-vessels-division-1/2017/print-book.

AspenTech. 2022a. “Aspen Plus.” 2022. https://www.aspentech.com/en/products/engineering/aspen-plus.

AspenTech. 2022b. “AspenTech | Asset Optimization Software - Asset Performance Management, Process Engineering for Chemicals, Energy and Engineering & Construction.” 2022. https://www.aspentech.com/en/.

AVEVA. 2022. “AVEVA PRO/II Simulation – The Trusted Steady-State Process Simulator.” 2022. https://www.aveva.com/en/products/pro-ii-simulation/.

Back, Thomas. 1991. “A Survey of Evolution Strategies.” In *Proc. 4th International Conference on Genetic Algorithms,(1991)*, 2–9.

Barlow, Jay, Ronald C. Sims, and Jason C. Quinn. 2016. “Techno-Economic and Life-Cycle Assessment of an Attached Growth Algal Biorefinery.” *Bioresource Technology* 220 (November): 360–68. https://doi.org/10.1016/j.biortech.2016.08.091.

BASF SE. 2020. “BASF Catalysts - Metal Prices.” 2020. https://apps.catalysts.basf.com/apps/eibprices/mp/defaultmain.aspx.

Bassano, Claudia, Paolo Deiana, Luca Lietti, and Carlo Giorgio Visconti. 2019. “P2G Movable Modular Plant Operation on Synthetic Methane Production from CO2 and Hydrogen from Renewables Sources.” *Fuel* 253 (October): 1071–79. https://doi.org/10.1016/j.fuel.2019.05.074.

Basu, Prabir. 2018. "Chapter 7 - Gasification Theory." In *Biomass Gasification, Pyrolysis and Torrefaction (Third Edition)*, edited by Prabir Basu, 211–62. Academic Press. https://doi.org/10.1016/B978-0-12-812992-0.00007-8.

Baten, Jasper van, and Michel Pons. 2014. "CAPE-OPEN: Interoperability in Industrial Flowsheet Simulation Software." *Chemie Ingenieur Technik* 86 (7): 1052–64. https://doi.org/10.1002/cite.201400009.

Beal, Colin M., Léda N. Gerber, Deborah L. Sills, Mark E. Huntley, Stephen C. Machesky, Michael J. Walsh, Jefferson W. Tester, Ian Archibald, Joe Granados, and Charles H. Greene. 2015. "Algal Biofuel Production for Fuels and Feed in a 100-Ha Facility: A Comprehensive Techno-Economic Analysis and Life Cycle Assessment." *Algal Research* 10 (July): 266–79. https://doi.org/10.1016/j.algal.2015.04.017.

Benoit Norris, C., S. Russo Garrido, M. Traverso, E. Ekener, S. Valdivia, A. Lehmann, and M. Finkbeiner. 2018. "A global effort: 2019 S-LCA guidelines." *Social LCA People and Places for partnership 6th SocSem Pre-proceeding, Fruitop Thema, Pescara*, 134–39.

Biscani, Francesco, and Dario Izzo. 2020. "A Parallel Global Multiobjective Framework for Optimization: Pagmo." *Journal of Open Source Software* 5 (53): 2338. https://doi.org/10.21105/joss.02338.

Boer, Harmen Sytze de, Lukas Grond, Henk Moll, and René Benders. 2014. "The Application of Power-to-Gas, Pumped Hydro Storage and Compressed Air Energy Storage in an Electricity System at Different Wind Power Penetration Levels." *Energy* 72 (August): 360–70. https://doi.org/10.1016/j.energy.2014.05.047.

Bradstreet, Lucas. 2011. *The Hypervolume Indicator for Multi-Objective Optimisation: Calculation and Use*. University of Western Australia Perth.

Brown, Tristan R, and Mark M Wright. 2014. "A Framework for Defining the Economic Feasibility of Cellulosic Biofuel Pathways." *Biofuels* 5 (5): 579–90. https://doi.org/10.1080/17597269.2014.1003700.

Capitanescu, F., S. Rege, A. Marvuglia, E. Benetto, A. Ahmadi, T. Navarrete Gutiérrez, and L. Tiruta-Barna. 2016. "Cost versus Life Cycle Assessment-Based Environmental Impact Optimization of Drinking Water Production Plants." *Journal of Environmental Management* 177 (July): 278–87. https://doi.org/10.1016/j.jenvman.2016.04.027.

Capitanescu, Florin, Antonino Marvuglia, Enrico Benetto, Aras Ahmadi, and Ligia Tiruta-Barna. 2016. *Constraint Programming versus MIP for LCA-Based Multi-Objective Optimization of Sustainable Potable Water Production Plants*.

CEC. 2001. "Green Paper on Integrated Product Policy."

CEC. 2013. "Communication from the Commission to the European Parliament and the Council. Building the Single Market for Green Products Facilitating Better Information on the Environmental Performance of Products and

Organisations." https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=celex%3A52013DC0196.

CEC. 2019. "Communication from the Commission to the European Parliament, the European Council, the Council, the European Economic and Social Committee and the Committee of the Regions. The European Green Deal."

CEC. 2020a. "Communication from the Commission to the European Parliament, the European Council, the Council, the European Economic and Social Committee and the Committee of the Regions. A New Industrial Strategy for Europe." https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A52020DC0102.

CEC. 2020b. "Communication from the Commission to the European Parliament, the European Council, the Council, the European Economic and Social Committee and the Committee of the Regions. The EU Budget Powering the Recovery Plan for Europe." https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A52020DC0442&qid=1657647455946.

Charnes, A., W. W. Cooper, and E. Rhodes. 1978. "Measuring the Efficiency of Decision Making Units." *European Journal of Operational Research* 2 (6): 429–44. https://doi.org/10.1016/0377-2217(78)90138-8.

Chiche, D., C. Diverchy, A.-C. Lucquin, F. Porcheron, and F. Defoort. 2013. "Synthesis Gas Purification." *Oil & Gas Science and Technology – Revue d'IFP Energies Nouvelles* 68 (4): 707–23. https://doi.org/10.2516/ogst/2013175.

Ciroth, Andreas, Gjalt Huppes, Walter Klöpffer, Ina Rüdenauer, Bengt Steen, and Thomas Swarr. 2008. *Environmental Life Cycle Costing*.

Clausen, Lasse R., Niels Houbak, and Brian Elmegaard. 2010. "Technoeconomic Analysis of a Methanol Plant Based on Gasification of Biomass and Electrolysis of Water." *Energy* 35 (5): 2338–47. https://doi.org/10.1016/j.energy.2010.02.034.

Collet, Pierre, Eglantine Flottes, Alain Favre, Ludovic Raynal, Hélène Pierre, Sandra Capela, and Carlos Peregrina. 2017. "Techno-Economic and Life Cycle Assessment of Methane Production via Biogas Upgrading and Power to Gas Technology." *Applied Energy* 192 (April): 282–95. https://doi.org/10.1016/j.apenergy.2016.08.181.

Cook, Wade D., and Larry M. Seiford. 2009. "Data Envelopment Analysis (DEA) – Thirty Years On." *European Journal of Operational Research* 192 (1): 1–17. https://doi.org/10.1016/j.ejor.2008.01.032.

Cormos, Calin-Cristian. 2011. "Evaluation of Power Generation Schemes Based on Hydrogen-Fuelled Combined Cycle with Carbon Capture and Storage (CCS)." *International Journal of Hydrogen Energy* 36 (5): 3726–38. https://doi.org/10.1016/j.ijhydene.2010.12.042.

Croxatto Vega, Giovanna, Joshua Sohn, Juliën Voogt, Morten Birkved, Stig Irving Olsen, and Anna Ekman Nilsson. 2021. "Insights from Combining Techno-Economic and Life Cycle Assessment – a Case Study of Polyphenol Extraction from Red Wine Pomace." *Resources, Conservation and Recycling* 167 (April): 105318. https://doi.org/10.1016/j.resconrec.2020.105318.

Croxatto Vega, Giovanna, Juliën Voogt, Joshua Sohn, Morten Birkved, and Stig Irving Olsen. 2020. “Assessing New Biotechnologies by Combining TEA and TM-LCA for an Efficient Use of Biomass Resources.” *Sustainability* 12 (9): 3676. https://doi.org/10.3390/su12093676.

Curran, Mary Ann. 1997. “Life-Cycle Based Government Policies a Survey.” *The International Journal of Life Cycle Assessment* 2 (1): 39. https://doi.org/10.1007/BF02978718.

Davis, R., L. Tao, E. C. D. Tan, M. J. Biddy, G. T. Beckham, C. Scarlata, J. Jacobson, et al. 2013. “Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons.” NREL/TP-5100-60223. National Renewable Energy Lab. (NREL), Golden, CO (United States). https://doi.org/10.2172/1107470.

Deb, K., A. Pratap, S. Agarwal, and T. Meyarivan. 2002. “A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II.” *IEEE Transactions on Evolutionary Computation* 6 (2): 182–97. https://doi.org/10.1109/4235.996017.

Deb, Kalyanmoy, Samir Agrawal, Amrit Pratap, and T. Meyarivan. 2000. “A Fast Elitist Non-Dominated Sorting Genetic Algorithm for Multi-Objective Optimization: NSGA-II.” In *Parallel Problem Solving from Nature PPSN VI*, edited by Marc Schoenauer, Kalyanmoy Deb, Günther Rudolph, Xin Yao, Evelyne Lutton, Juan Julian Merelo, and Hans-Paul Schwefel, 849–58. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer. https://doi.org/10.1007/3-540-45356-3_83.

DeRose, Katherine, Chad DeMill, Ryan W. Davis, and Jason C. Quinn. 2019. “Integrated Techno Economic and Life Cycle Assessment of the Conversion of High Productivity, Low Lipid Algae to Renewable Fuels.” *Algal Research* 38 (March): 101412. https://doi.org/10.1016/j.algal.2019.101412.

Diamantopoulou, L. K., L. S. Karaoglanoglou, and E. G. Koukios. 2011. “Biomass Cost Index: Mapping Biomass-to-Biohydrogen Feedstock Costs by a New Approach.” *Bioresource Technology* 102 (3): 2641–50. https://doi.org/10.1016/j.biortech.2010.10.102.

Dimian, Alexandre C., Costin S. Bildea, and Anton A. Kiss. 2014. “Chapter 2 - Introduction in Process Simulation.” In *Computer Aided Chemical Engineering*, edited by Alexandre C. Dimian, Costin S. Bildea, and Anton A. Kiss, 35:35–71. Integrated Design and Simulation of Chemical Processes. Elsevier. https://doi.org/10.1016/B978-0-444-62700-1.00002-4.

Directive (EU) 2018/2001 of the European Parliament and of the Council of 11 December 2018 on the Promotion of the Use of Energy from Renewable Sources (Recast) (Text with EEA Relevance.). 2018. *OJ L*. Vol. 328. http://data.europa.eu/eli/dir/2018/2001/oj/eng.

Dry, Mark E. 2002. “The Fischer–Tropsch Process: 1950–2000.” *Catalysis Today*, Fischer-Tropsch synthesis on the eve of the XXI Century, 71 (3): 227–41. https://doi.org/10.1016/S0920-5861(01)00453-9.

Dupont, Capucine, Rodica Chiriac, Guillaume Gauthier, and François Toche. 2014. “Heat Capacity Measurements of Various Biomass Types and Pyrolysis Residues.” *Fuel* 115 (January): 644–51. https://doi.org/10.1016/j.fuel.2013.07.086.

EC. 1992. “Council Regulation (EEC) No 880/92 of 23 March 1992 on a Community Eco-Label Award Scheme.” https://eur-lex.europa.eu/legal-content/LT/TXT/?uri=CELEX%3A31992R0880.

EC. 2009. *Directive 2009/125/EC of the European Parliament and of the Council of 21 October 2009 Establishing a Framework for the Setting of Ecodesign Requirements for Energy-Related Products (Text with EEA Relevance)*. *OJ L*. http://data.europa.eu/eli/dir/2009/125/oj/eng.

EC. 2010. *Regulation (EC) No 66/2010 of the European Parliament and of the Council of 25 November 2009 on the EU Ecolabel*. *OJ L*. Vol. 027. http://data.europa.eu/eli/reg/2010/66/oj/eng.

EC. 2013. “Commission Recommendation of 9 April 2013 on the Use of Common Methods to Measure and Communicate the Life Cycle Environmental Performance of Products and Organisations.” *OJ L*. Vol. 124. http://data.europa.eu/eli/reco/2013/179/oj/eng.

EC. 2021. *Regulation (EU) 2021/241 of the European Parliament and of the Council of 12 February 2021 Establishing the Recovery and Resilience Facility*. *OJ L*. Vol. 057. http://data.europa.eu/eli/reg/2021/241/oj/eng.

EC. 2022. “European Platform on Life Cycle Assessment (LCA).” 2022. https://ec.europa.eu/environment/ipp/lca.htm.

Ekener Petersen, E. 2015. “State of the art on social LCA.” *Social Life Cycle Assessment-State of the Art and Challenges for Supporting Product Policies*, 27–31.

Elsayed, Saber M., Ruhul A. Sarker, and Daryl L. Essam. 2011. “Differential Evolution with Multiple Strategies for Solving CEC2011 Real-World Numerical Optimization Problems.” In *2011 IEEE Congress of Evolutionary Computation (CEC)*, 1041–48. https://doi.org/10.1109/CEC.2011.5949732.

European Commission. 2013. “2 Million Tons per Year: A Performing Biofuels Supply Chain for EU Aviation (Technical Report).”

Ferrara, G., A. Lanzini, P. Leone, M. T. Ho, and D. E. Wiley. 2017. “Exergetic and Exergoeconomic Analysis of Post-Combustion CO2 Capture Using MEA-Solvent Chemical Absorption.” *Energy* 130 (July): 113–28. https://doi.org/10.1016/j.energy.2017.04.096.

Frischknecht, Rolf, Niels Jungbluth, Hans-Jörg Althaus, Gabor Doka, Roberto Dones, Thomas Heck, Stefanie Hellweg, et al. 2005. “The Ecoinvent Database: Overview and Methodological Framework (7 Pp).” *The International Journal of Life Cycle Assessment* 10 (1): 3–9. https://doi.org/10.1065/lca2004.10.181.1.

Gabathuler, Heinz. 2006. “The CML Story: How Environmental Sciences Entered the Debate on LCA.” *The International Journal of Life Cycle Assessment* 11 (1): 127–32. https://doi.org/10.1065/lca2006.04.021.

Glacier Media Group. 2020. “Markets Single - MINING.COM.” 2020. https://www.mining.com/markets/commodity/ruthenium/.

GLAD. 2023. “Global LCA Data Access Network.” 2023. https://www.globallcadataaccess.org/.

Gluch, Pernilla, and Henrikke Baumann. 2004. “The Life Cycle Costing (LCC) Approach: A Conceptual Discussion of Its Usefulness for Environmental Decision-Making.” *Building and Environment* 39 (5): 571–80. https://doi.org/10.1016/j.buildenv.2003.10.008.

Gnanamani, Muthu Kumaran, Wilson D. Shafer, Dennis E. Sparks, and Burtron H. Davis. 2011. “Fischer–Tropsch Synthesis: Effect of CO2 Containing Syngas over Pt Promoted Co/γ-Al2O3 and K-Promoted Fe Catalysts.” *Catalysis Communications* 12 (11): 936–39. https://doi.org/10.1016/j.catcom.2011.03.002.

Goedkoop, Mark, and R. Spriensma. 2001. “The Eco-Indicator 99: A Damage Oriented Method for Life Cycle Impact Assessment,” January.

Götz, Manuel, Jonathan Lefebvre, Friedemann Mörs, Amy McDaniel Koch, Frank Graf, Siegfried Bajohr, Rainer Reimert, and Thomas Kolb. 2016. “Renewable Power-to-Gas: A Technological and Economic Review.” *Renewable Energy* 85 (January): 1371–90. https://doi.org/10.1016/j.renene.2015.07.066.

GreenDelta. 2022. “OpenLCA.” https://www.openlca.org/.

Guinée, J.B., M. Gorrée, Reinout Heijungs, Gjalt Huppes, Rene Kleijn, Lauran Oers, Anneke Wegener Sleeswijk, et al. 2001. “Life Cycle Assessment: An Operational Guide to ISO Standards.” *Life Cycle Assessment: An Operational Guide to ISO Standards* 1 (January).

Guinée, Jeroen. 2016. “Life Cycle Sustainability Assessment: What Is It and What Are Its Challenges?” In *Taking Stock of Industrial Ecology*, edited by Roland Clift and Angela Druckman, 45–68. Cham: Springer International Publishing. https://doi.org/10.1007/978-3-319-20571-7_3.

Hamelinck, Carlo N., André P. C. Faaij, Herman den Uil, and Harold Boerrigter. 2004. “Production of FT Transportation Fuels from Biomass; Technical Options, Process Analysis and Optimisation, and Development Potential.” *Energy* 29 (11): 1743–71. https://doi.org/10.1016/j.energy.2004.01.002.

Hammond, Mark. 2022. “Pywin32.” https://github.com/mhammond/pywin32.

Hanaoka, Toshiaki, Tomohisa Miyazawa, Katsuya Shimura, and Satoshi Hirata. 2015. “Jet Fuel Synthesis from Fischer–Tropsch Product under Mild Hydrocracking Conditions Using Pt-Loaded Catalysts.” *Chemical Engineering Journal* 263 (March): 178–85. https://doi.org/10.1016/j.cej.2014.11.042.

Harris, Charles R., K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, et al. 2020. “Array Programming with NumPy.” *Nature* 585 (7825): 357–62. https://doi.org/10.1038/s41586-020-2649-2.

Haydary, Juma. 2019. *Chemical Process Design and Simulation: Aspen Plus and Aspen Hysys Applications*. https://www.wiley.com/en-us/Chemical+Process+Design+and+Simulation%3A+Aspen+Plus+and+Aspen+Hysys+Applications-p-9781119089117.

Heijungs, Reinout, and Sangwon Suh. 2002. *The Computational Structure of Life Cycle Assessment*. Vol. 11. Eco-Efficiency in Industry and Science. Dordrecht: Springer Netherlands. https://doi.org/10.1007/978-94-015-9900-9.

Hellweg, Stefanie, and Llorenç Milà i Canals. 2014. "Emerging Approaches, Challenges and Opportunities in Life Cycle Assessment." *Science* 344 (6188): 1109–13. https://doi.org/10.1126/science.1248361.

Hertwich, Edgar G. 2005. "Life Cycle Approaches to Sustainable Consumption: A Critical Review." *Environmental Science & Technology* 39 (13): 4673–84. https://doi.org/10.1021/es0497375.

Hise, Adam M., Gregory W. Characklis, Jordan Kern, Robin Gerlach, Sridhar Viamajala, Robert D. Gardner, and Agasteswar Vadlamani. 2016. "Evaluating the Relative Impacts of Operational and Financial Factors on the Competitiveness of an Algal Biofuel Production Facility." *Bioresource Technology* 220 (November): 271–81. https://doi.org/10.1016/j.biortech.2016.08.050.

Holmgren, Kristina. 2015. "Investment Cost Estimates for Gasification-Based Biofuel Production Systems." IVL Svenska Miljöinstitutet.

Huijbregts, Mark, ZJN Steinmann, PMF Elshout, G Stam, F Verones, MDM Vieira, A Hollander, and R Van Zelm. 2016. "ReCiPe 2016: A Harmonized Life Cycle Impact Assessment Method at Midpoint and Endpoint Level." RIVM Report. Bilthoven, The Netherlands.

Hunkeler, David, Kerstin Lichtenvort, and Gerald Rebitzer. 2008. *Environmental Life Cycle Costing*. Crc press.

Hunter, J. D. 2007. "Matplotlib: A 2D Graphics Environment." *Computing in Science & Engineering* 9 (3): 90–95. https://doi.org/10.1109/MCSE.2007.55.

Hwang, Ching-Lai, and Kwangsun Yoon. 1981. *Multiple Attribute Decision Making*. https://link.springer.com/book/10.1007/978-3-642-48318-9.

IDAE. 2019. "Informe de Precios de La Biomasa Para Usos Térmicos (Technical Report)."

Inc, Plotly Technologies. 2015. "Collaborative Data Science." Montreal, QC: Plotly Technologies Inc. 2015. https://plot.ly.

iPoint. 2022. "Eco-Efficiency Software – Umberto." 2022. https://www.ifu.com/.

Iribarren, Diego, Ana Susmozas, and Javier Dufour. 2013. "Life-Cycle Assessment of Fischer–Tropsch Products from Biosyngas." *Renewable Energy* 59 (November): 229–36. https://doi.org/10.1016/j.renene.2013.04.002.

ISO. 2006a. "ISO 14040: Environmental Management — Life Cycle Assessment — Principles and Framework." Geneva, Switzerland: International Organization for Standardization.

https://www.iso.org/cms/render/live/en/sites/isoorg/contents/data/standard/03/74/37456.html.

ISO. 2006b. "ISO 14044: Environmental Management — Life Cycle Assessment — Requirements and Guidelines." Geneva, Switzerland: International Organization for Standardization. https://www.iso.org/cms/render/live/en/sites/isoorg/contents/data/standard/03/84/38498.html.

ISO. 2017. "ISO 15686-5: Buildings and Constructed Assets — Service-Life Planning — Part 5: Life-Cycle Costing." https://www.iso.org/cms/render/live/en/sites/isoorg/contents/data/standard/03/98/39843.html.

ISO. 2021. "ISO 15663: Petroleum, Petrochemical and Natural Gas Industries — Life Cycle Costing." https://www.iso.org/cms/render/live/en/sites/isoorg/contents/data/standard/07/91/79198.html.

Jenkins, Scott. 2022. "Plant Cost Index Archives." *Chemical Engineering* (blog). 2022. https://www.chemengonline.com/site/plant-cost-index/.

Joint Research Centre, Eckehard Rosenbaum, Lucia Mancini, Alessandro Vasta, Serenella Sala, and Jo Dewulf. 2015. *Social Life Cycle Assessment: State of the Art and Challenges for Product Policy Support*. LU: Publications Office of the European Union. https://data.europa.eu/doi/10.2788/253715.

Jolliet, Olivier, Manuele Margni, Raphaël Charles, Sébastien Humbert, Jerome Payet, Gerald Rebitzer, and Ralph Rosenbaum. 2003. "IMPACT 2002+: A New Life Cycle Assessment Methodology. Int J Life Cycle Assess 8:324-330." *The International Journal of Life Cycle Assessment* 8 (November): 324–30. https://doi.org/10.1007/BF02978505.

Kalbar, Pradip P., and Deepjyoti Das. 2020. "Chapter 10 - Advancing Life Cycle Sustainability Assessment Using Multiple Criteria Decision Making." In *Life Cycle Sustainability Assessment for Decision-Making*, edited by Jingzheng Ren and Sara Toniolo, 205–24. Elsevier. https://doi.org/10.1016/B978-0-12-818355-7.00010-5.

Karn, F. S., J. F. Schultz, R. E. Kelly, and R. B. Anderson. 1963. "Fischer-Tropsch Synthesis. Poisoning of Iron Catalysts by H2S in Synthesis Gas." *I&EC Product Research and Development* 2 (1): 43–47. https://doi.org/10.1021/i360005a011.

Kennedy, J., and R. Eberhart. 1995. "Particle Swarm Optimization." In *Proceedings of ICNN'95 - International Conference on Neural Networks*, 4:1942–48 vol.4. https://doi.org/10.1109/ICNN.1995.488968.

Kent, James A. 2007. *Kent and Riegel's Handbook of Industrial Chemistry and Biotechnology*. https://link.springer.com/book/10.1007/978-0-387-27843-8.

Khoshnevisan, Benyamin, Elham Bolandnazar, Shahaboddin Shamshirband, Hanifreza Motamed Shariati, Nor Badrul Anuar, and Miss Laiha Mat Kiah. 2015. "Decreasing Environmental Impacts of Cropping Systems Using Life Cycle

Assessment (LCA) and Multi-Objective Genetic Algorithm." *Journal of Cleaner Production* 86 (January): 67–77. https://doi.org/10.1016/j.jclepro.2014.08.062.

KLM Technology. 2013. "Engineering Design Guidelines (Technical Report)."

Kloepffer, Walter. 2008. "Life Cycle Sustainability Assessment of Products." *The International Journal of Life Cycle Assessment* 13 (2): 89. https://doi.org/10.1065/lca2008.02.376.

Kopyscinski, Jan. 2010. "Production of Synthetic Natural Gas in a Fluidized Bed Reactor: Understanding the Hydrodynamic, Mass Transfer, and Kinetic Effects." Doctoral Thesis, ETH Zurich. https://doi.org/10.3929/ethz-a-006031831.

Lappas, A., and E. Heracleous. 2016. "18 - Production of Biofuels via Fischer–Tropsch Synthesis: Biomass-to-Liquids." In *Handbook of Biofuels Production (Second Edition)*, edited by Rafael Luque, Carol Sze Ki Lin, Karen Wilson, and James Clark, 549–93. Woodhead Publishing. https://doi.org/10.1016/B978-0-08-100455-5.00018-7.

LCI-webteam. "What Is Life Cycle Thinking?" *Life Cycle Initiative* (blog). Accessed May 9, 2022. https://www.lifecycleinitiative.org/starting-life-cycle-thinking/what-is-life-cycle-thinking/.

Leibbrandt, Nadia H., Akinwale O. Aboyade, Johannes H. Knoetze, and Johann F. Görgens. 2013. "Process Efficiency of Biofuel Production via Gasification and Fischer–Tropsch Synthesis." *Fuel* 109 (July): 484–92. https://doi.org/10.1016/j.fuel.2013.03.013.

Li, Hui, and Qingfu Zhang. 2009. "Multiobjective Optimization Problems With Complicated Pareto Sets, MOEA/D and NSGA-II." *IEEE Transactions on Evolutionary Computation* 13 (2): 284–302. https://doi.org/10.1109/TEVC.2008.925798.

Li, Jia, Samuel Feaster, and Andrew Kohler. 2019. "A Multi-Objective Multi-Technology (MOMT) Evaluation and Analysis Framework for Ammonia Synthesis Process Development." In *Computer Aided Chemical Engineering*, edited by Salvador Garcia Muñoz, Carl D. Laird, and Matthew J. Realff, 47:415–20. Proceedings of the 9 International Conference on Foundations of Computer-Aided Process Design. Elsevier. https://doi.org/10.1016/B978-0-12-818597-1.50066-7.

Li, Xiaodong. 2003. "A Non-Dominated Sorting Particle Swarm Optimizer for Multiobjective Optimization." In *Genetic and Evolutionary Computation — GECCO 2003*, edited by Erick Cantú-Paz, James A. Foster, Kalyanmoy Deb, Lawrence David Davis, Rajkumar Roy, Una-May O'Reilly, Hans-Georg Beyer, et al., 37–48. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer. https://doi.org/10.1007/3-540-45105-6_4.

Livingstone, David J. 2008. *Artificial Neural Networks: Methods and Applications: 458*. Totowa, NJ.

Lohman, Egan, Rob Gardner, Todd Pedersen, Brent Peyton, Keith Cooksey, and Robin Gerlach. 2015. "Optimized Inorganic Carbon Regime for Enhanced Growth and

Lipid Accumulation in Chlorella Vulgaris Luisa Gouveia." *Biotechnology for Biofuels* 8 (December): 82. https://doi.org/10.1186/s13068-015-0265-4.

López-Andrés, Jhony Josué, Alberto Alfonso Aguilar-Lasserre, Luis Fernando Morales-Mendoza, Catherine Azzaro-Pantel, Jorge Raúl Pérez-Gallardo, and José Octavio Rico-Contreras. 2018. "Environmental Impact Assessment of Chicken Meat Production via an Integrated Methodology Based on LCA, Simulation and Genetic Algorithms." *Journal of Cleaner Production* 174 (February): 477–91. https://doi.org/10.1016/j.jclepro.2017.10.307.

Ma, Xiaoliang, Qingfu Zhang, Guangdong Tian, Junshan Yang, and Zexuan Zhu. 2018. "On Tchebycheff Decomposition Approaches for Multiobjective Evolutionary Optimization." *IEEE Transactions on Evolutionary Computation* 22 (2): 226–44. https://doi.org/10.1109/TEVC.2017.2704118.

Mafakheri, Fereshteh, and Fuzhan Nasiri. 2014. "Modeling of Biomass-to-Energy Supply Chain Operations: Applications, Challenges and Research Directions." *Energy Policy* 67 (April): 116–26. https://doi.org/10.1016/j.enpol.2013.11.071.

Mahmud, Roksana, Sheikh Moniruzzaman Moni, Karen High, and Michael Carbajales-Dale. 2021. "Integration of Techno-Economic Analysis and Life Cycle Assessment for Sustainable Process Design – A Review." *Journal of Cleaner Production* 317 (October): 128247. https://doi.org/10.1016/j.jclepro.2021.128247.

Maia de Souza, Danielle, Tiago Braga, Maria Cléa Brito de Figueirêdo, Marília I. S. Folegatti Matsuura, Fernando Rodrigues Teixeira Dias, and Cássia Maria Lie Ugaya. 2017. "Life Cycle Thinking in Brazil: Challenges and Advances towards a More Comprehensive Practice." *The International Journal of Life Cycle Assessment* 22 (3): 462–65. https://doi.org/10.1007/s11367-016-1234-2.

Masson-Delmotte, Valérie, Panmao Zhai, Anna Pirani, Sarah L. Connors, Clotilde Péan, Sophie Berger, Nada Caud, et al., eds. 2021. *Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*. Cambridge, United Kingdom and New York, NY, USA: Cambridge University Press. https://doi.org/10.1017/9781009157896.

Mazzi, Anna. 2020. "Chapter 1 - Introduction. Life Cycle Thinking." In *Life Cycle Sustainability Assessment for Decision-Making*, edited by Jingzheng Ren and Sara Toniolo, 1–19. Elsevier. https://doi.org/10.1016/B978-0-12-818355-7.00001-4.

McCord, Stephen, Ana Villa Zaragoza, Peter Styring, Lorenzo Cremonese, Yuan Wang, Tim Langhorst, and Volker Sick. 2021. "Multi-Attributional Decision Making in LCA & TEA for CCU: An Introduction to Approaches and a Worked Example." Technical Report. Global CO2 Initiative. https://doi.org/10.7302/805.

McCoy, Sean T, and Edward S Rubin. 2005. "Models of CO2 Transport and Storage Costs and Their Importance in CCS Cost Estimates."

Mencarelli, Luca, Alexandre Pagot, and Pascal Duchêne. 2020. "Surrogate-Based Modeling Techniques with Application to Catalytic Reforming and Isomerization

Processes." *Computers & Chemical Engineering* 135 (April): 106772. https://doi.org/10.1016/j.compchemeng.2020.106772.

Méndez, César I., and Jorge Ancheyta. 2020. "Modeling and Control of a Fischer-Tropsch Synthesis Fixed-Bed Reactor with a Novel Mechanistic Kinetic Approach." *Chemical Engineering Journal* 390 (June): 124489. https://doi.org/10.1016/j.cej.2020.124489.

Mernik, Marjan, Shih-Hsi Liu, Dervis Karaboga, and Matej Črepinšek. 2015. "On Clarifying Misconceptions When Comparing Variants of the Artificial Bee Colony Algorithm by Offering a New Implementation." *Information Sciences* 291 (January): 115–27. https://doi.org/10.1016/j.ins.2014.08.040.

Mery, Yoann, Ligia Tiruta-Barna, Enrico Benetto, and Isabelle Baudin. 2013. "An Integrated Process Modelling-Life Cycle Assessment Tool for the Assessment and Design of Water Treatment Processes." *The International Journal of Life Cycle Assessment* 18 (June): 1062–70. https://doi.org/10.1007/s11367-012-0541-5.

Miller, Nathan, Adam Christensen, Ji Eun Park, Anil Baral, Chris Malins, and Stephanie Searle. 2013. "Measuring and Addressing Investment Risk in the Second-Generation Biofuels Industry." *International Council on Clean Transportation*. https://theicct.org/publication/measuring-and-addressing-investment-risk-in-the-second-generation-biofuels-industry/.

Ministerio para la Transición Ecológica. 2018. "Resolución de 8 de octubre de 2018, de la Dirección General de Política Energética y Minas, por la que se modifican las normas de gestión técnica del sistema NGTS-06, NGTS-07 y los protocolos de detalle PD-01 y PD-02." 256. BOE. https://www.boe.es/eli/es/res/2018/10/08/(3).

Mirghaderi, Seyed Davoud, and Mahmoud Modiri. 2021. "Application of Meta-Heuristic Algorithm for Multi-Objective Optimization of Sustainable Supply Chain Uncertainty." *Sādhanā* 46 (1): 52. https://doi.org/10.1007/s12046-020-01554-4.

Moioli, Emanuele, Noris Gallandat, and Andreas Züttel. 2019. "Model Based Determination of the Optimal Reactor Concept for Sabatier Reaction in Small-Scale Applications over Ru/Al2O3." *Chemical Engineering Journal* 375 (November): 121954. https://doi.org/10.1016/j.cej.2019.121954.

MongoDB. 2022. "MongoDB." https://www.mongodb.com.

MongoDB. 2022. "PyMongo." Python. mongodb. https://github.com/mongodb/mongo-python-driver.

Moni, Sheikh Moniruzzaman, Roksana Mahmud, Karen High, and Michael Carbajales-Dale. 2020. "Life Cycle Assessment of Emerging Technologies: A Review." *Journal of Industrial Ecology* 24 (1): 52–63. https://doi.org/10.1111/jiec.12965.

Morris, Max D. 1991. "Factorial Sampling Plans for Preliminary Computational Experiments." *Technometrics* 33 (2): 161–74. https://doi.org/10.2307/1269043.

Mortensen, Peter Mølgaard, and Ib Dybkjær. 2015. "Industrial Scale Experience on Steam Reforming of CO2-Rich Gas." *Applied Catalysis A: General* 495 (April): 141–51. https://doi.org/10.1016/j.apcata.2015.02.022.

Murata, T., and H. Ishibuchi. 1995. "MOGA: Multi-Objective Genetic Algorithms." In *Proceedings of 1995 IEEE International Conference on Evolutionary Computation*, 1:289-. https://doi.org/10.1109/ICEC.1995.489161.

Mutel, Chris. 2017. "Brightway: An Open Source Framework for Life Cycle Assessment." *Journal of Open Source Software* 2 (12): 236. https://doi.org/10.21105/joss.00236.

National Renewable Energy Laboratory (NREL). 2012. "Current State-of-the-Art Hydrogen Production Cost Estimate Using Water Electrolysis: Independent Review."

NREL. 2012. "U.S. Life Cycle Inventory Database." 2012. https://www.lcacommons.gov/nrel/search.

Nuss, Philip, and Matthew J. Eckelman. 2014. "Life Cycle Assessment of Metals: A Scientific Synthesis." *PLOS ONE* 9 (7): e101298. https://doi.org/10.1371/journal.pone.0101298.

Opricovic, Serafim, and Gwo-Hshiung Tzeng. 2004. "Compromise Solution by MCDM Methods: A Comparative Analysis of VIKOR and TOPSIS." *European Journal of Operational Research* 156 (2): 445–55. https://doi.org/10.1016/S0377-2217(03)00020-1.

Panwar, Abhilasha, Kamalendra Kumar Tripathi, and Kumar Neeraj Jha. 2019. "A Qualitative Framework for Selection of Optimization Algorithm for Multi-Objective Trade-off Problem in Construction Projects." *Engineering, Construction and Architectural Management* 26 (9): 1924–45. https://doi.org/10.1108/ECAM-06-2018-0246.

Parkhurst, David L., and C. A. J. Apello. 2014. *Description of Input and Examples for PHREEQC Version 3?A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations*.

Peano, Laura, An De Schryver, Sebastien Humbert, Yves Loerincik, Gérard Gaillard, Jens Lansche, and Thomas Nemecek. 2012. "The World Food LCA Database Project: Towards More Accurate Food Datasets." In . Lille, France.

Pennington, David, Marc-Andree Wolf, Raffaella Bersani, and Ugo Pretato. 2007. "Overcoming Barriers to the Broader Implementation of Life Cycle Thinking in Business and Public Administration." *The International Journal of Life Cycle Assessment* 12 (7): 458. https://doi.org/10.1065/lca2007.07.355.

Powell, M. J. D. 1998. "Direct Search Algorithms for Optimization Calculations." *Acta Numerica* 7 (January): 287–336. https://doi.org/10.1017/S0962492900002841.

PRé Sustainability. 2022. "SimaPro." https://simapro.com/.

Price, Kenneth, Rainer M. Storn, and Jouni A. Lampinen. 2005. *Differential Evolution: A Practical Approach to Global Optimization*. Berlin ; New York.

Python Software Foundation. 2022. “Python.Org.” Python.Org. 2022. https://www.python.org/.

Rafati, Mohammad, Lijun Wang, David C. Dayton, Keith Schimmel, Vinayak Kabadi, and Abolghasem Shahbazi. 2017. “Techno-Economic Analysis of Production of Fischer-Tropsch Liquids via Biomass Gasification: The Effects of Fischer-Tropsch Catalysts and Natural Gas Co-Feeding.” *Energy Conversion and Management* 133 (February): 153–66. https://doi.org/10.1016/j.enconman.2016.11.051.

Reed, Daniel L. 2012. “Life-Cycle Assessment in Government Policy in the United States.” Knoxville: University of Tennessee.

Regulation (EU) 2017/2392 of the European Parliament and of the Council of 13 December 2017 Amending Directive 2003/87/EC to Continue Current Limitations of Scope for Aviation Activities and to Prepare to Implement a Global Market-Based Measure from 2021. 2017. *OJ L*. Vol. 350. http://data.europa.eu/eli/reg/2017/2392/oj/eng.

Rivarolo, M., L. Magistri, and A. F. Massardo. 2014. “Hydrogen and Methane Generation from Large Hydraulic Plant: Thermo-Economic Multi-Level Time-Dependent Optimization.” *Applied Energy* 113 (January): 1737–45. https://doi.org/10.1016/j.apenergy.2013.08.072.

Rüdenauer, Ina, Carl-Otto Gensch, Rainer Grießhammer, and Dirk Bunke. 2005. “Integrated Environmental and Economic Assessment of Products and Processes.” *Journal of Industrial Ecology* 9 (October): 105–16. https://doi.org/10.1162/108819805775248061.

Saaty, R. W. 1987a. “The Analytic Hierarchy Process—What It Is and How It Is Used.” *Mathematical Modelling* 9 (3–5): 161–76. https://doi.org/10.1016/0270-0255(87)90473-8.

Saaty, R. W. 1987b. “The Analytic Hierarchy Process—What It Is and How It Is Used.” *Mathematical Modelling* 9 (3): 161–76. https://doi.org/10.1016/0270-0255(87)90473-8.

Sabatier, P, and JB Senderens. 1902. “Comptes Rendus Des Séances De L’Académie Des Sciences, Section VI–Chimie.” *Paris: Imprimerie Gauthier-Villars*.

Sala, Serenella, Andrea Martino Amadei, Antoine Beylot, and Fulvio Ardente. 2021. “The Evolution of Life Cycle Assessment in European Policies over Three Decades.” *The International Journal of Life Cycle Assessment* 26 (12): 2295–2314. https://doi.org/10.1007/s11367-021-01893-2.

Samborskaya, M. A., V. P. Gusev, I. A. Gryaznova, N. S. Vdovushkina, and A. V. Volf. 2014. “Crude Oil Distillation with Superheated Water Steam: Parametrical Sensitivity and Optimization.” *Procedia Chemistry*, XV International Scientific Conference “Chemistry and Chemical Engineering in XXI century” dedicated to Professor L.P. Kulyov, 10 (January): 337–42. https://doi.org/10.1016/j.proche.2014.10.057.

Santos, Ronaldo Gonçalves dos, and Andre Cardoso Alencar. 2020. “Biomass-Derived Syngas Production via Gasification Process and Its Catalytic Conversion into

Fuels by Fischer Tropsch Synthesis: A Review." *International Journal of Hydrogen Energy*, Waste and Biomass-derived Hydrogen Synthesis and Implementation, 45 (36): 18114–32. https://doi.org/10.1016/j.ijhydene.2019.07.133.

Schlüter, Martin, Jose A. Egea, and Julio R. Banga. 2009. "Extended Ant Colony Optimization for Non-Convex Mixed Integer Nonlinear Programming." *Computers & Operations Research* 36 (7): 2217–29. https://doi.org/10.1016/j.cor.2008.08.015.

Scott, J. Alexander, and Thomas A. Adams II. 2018. "Biomass-Gas-and-Nuclear-to-Liquids (BGNTL) Processes Part I: Model Development and Simulation." *The Canadian Journal of Chemical Engineering* 96 (9): 1853–71. https://doi.org/10.1002/cjce.23231.

SETAC. 1994. "Guidelines for Life-Cycle Assessment:" *Environmental Science and Pollution Research* 1 (1): 55–55. https://doi.org/10.1007/BF02986927.

Shakoor, Zaidoon M. 2011. "CATALYTIC REFORMING OF HEAVY NAPHTHA, ANALYSIS AND SIMULATION." *Diyala Journal of Engineering Sciences* 4 (2): 86–104. https://doi.org/10.24237/djes.2011.04207.

Silva, Diogo, Andréa Nunes, Virgínia Moris, Cassiano Piekarski, and Thiago Rodrigues. 2017. *How Important Is the LCA Software Tool You Choose Comparative Results from GaBi, OpenLCA, SimaPro and Umberto*.

Sims, Ralph E. H., Warren Mabee, Jack N. Saddler, and Michael Taylor. 2010. "An Overview of Second Generation Biofuel Technologies." *Bioresource Technology* 101 (6): 1570–80. https://doi.org/10.1016/j.biortech.2009.11.046.

Sohn, Joshua, Pierre Bisquert, Patrice Buche, Abdelraouf Hecham, Pradip P. Kalbar, Ben Goldstein, Morten Birkved, and Stig Irving Olsen. 2020. "Argumentation Corrected Context Weighting-Life Cycle Assessment: A Practical Method of Including Stakeholder Perspectives in Multi-Criteria Decision Support for LCA." *Sustainability* 12 (6): 2170. https://doi.org/10.3390/su12062170.

Sohn, Joshua, Giovanna Croxatto Vega, and Morten Birkved. 2018. "A Methodology Concept for Territorial Metabolism – Life Cycle Assessment: Challenges and Opportunities in Scaling from Urban to Territorial Assessment." *Procedia CIRP*, 25th CIRP Life Cycle Engineering (LCE) Conference, 30 April – 2 May 2018, Copenhagen, Denmark, 69 (January): 89–93. https://doi.org/10.1016/j.procir.2017.10.005.

Soltanpour, Y., I. Peri, and L. Temri. 2018. "Discussing features of social measures important in SLCA impact indicators' selection." *Social LCA People and Places for Partnership 6th SocSem Pre-Proceeding, Fruitop Thema, Pescara*, 52–56.

Sönke Bröcker, Regina Benfer, Michael Bortz, Sebastian Engell, Carsten Knösche, and Andreas Kröner. 2021. "Process Simulation - Fit for the Future?" Dechema. https://dechema.de/en/Positionspapier_Prozesssimulation/_/PP_Process_Simulation_2021_engl.pdf.

Sonnemann, G., E. D. Gemechu, S. Sala, E. M. Schau, K. Allacker, R. Pant, N. Adibi, and S. Valdivia. 2018. "Life Cycle Thinking and the Use of LCA in Policies Around the World." In *Life Cycle Assessment: Theory and Practice*, edited by Michael Z. Hauschild, Ralph K. Rosenbaum, and Stig Irving Olsen, 429–63. Cham: Springer International Publishing. https://doi.org/10.1007/978-3-319-56475-3_18.

Souza-Santos, Marcio L. de. 2010. *Solid Fuels Combustion and Gasification: Modeling, Simulation, and Equipment Operations Second Edition*. 2nd ed. Boca Raton: CRC Press. https://doi.org/10.1201/9781420047509.

SQLite Consortium. 2022. "SQLite." https://www.sqlite.org/index.html.

Steynberg, André P, and Herman G Nel. 2004. "Clean Coal Conversion Options Using Fischer–Tropsch Technology." *Fuel*, Clean coal technology, 83 (6): 765–70. https://doi.org/10.1016/j.fuel.2003.09.023.

Stocker, T.F., D. Qin, G.K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex, and P.M. Midgley. 2013. "Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change." Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA: IPCC. https://www.ipcc.ch/report/ar5/wg1/.

Susmozas, Ana. 2015. "Análisis de sistemas energéticos basados en gasificación de biomasa." https://eciencia.urjc.es/handle/10115/13599.

Swanson, R. M., A. Platon, J. A. Satrio, R. C. Brown, and D. D. Hsu. 2010. "Techno-Economic Analysis of Biofuels Production Based on Gasification." NREL/TP-6A20-46587. National Renewable Energy Lab. (NREL), Golden, CO (United States). https://doi.org/10.2172/994017.

Tawarmalani, Mohit, and Nikolaos V. Sahinidis. 2005. "A Polyhedral Branch-and-Cut Approach to Global Optimization." *Mathematical Programming* 103 (2): 225–49. https://doi.org/10.1007/s10107-005-0581-8.

The London Metal Exchange - an HKEX Company. 2020. "LME Alumina (Platts) | London Metal Exchange." Lme. 2020. https://www.lme.com/Metals/Non-ferrous/LME-Alumina.

Thomassen, Gwenny, Miet Van Dael, Steven Van Passel, and Fengqi You. 2019. "How to Assess the Potential of Emerging Green Technologies? Towards a Prospective Environmental and Techno-Economic Assessment Framework." *Green Chemistry* 21 (18): 4868–86. https://doi.org/10.1039/C9GC02223F.

Tijmensen, Michiel J. A., André P. C. Faaij, Carlo N. Hamelinck, and Martijn R. M. van Hardeveld. 2002. "Exploration of the Possibilities for Production of Fischer Tropsch Liquids and Power via Biomass Gasification." *Biomass and Bioenergy* 23 (2): 129–52. https://doi.org/10.1016/S0961-9534(02)00037-5.

Tischner, Ursula, Eva Schmincke, Frieder Rubik, Martin Prosler, and German Federal Environmental Agency. 2000. *How to Do Ecodesign?: A Guide for Environmentally and Economically Sound Design*. Frankfurt am Main.

TNO Biobased and Circular Technologies. 2020. "Phyllis2, Database for (Treated) Biomass, Algae, Feedstocks for Biogas Production and Biochar." https://phyllis.nl/.

Towler, Gavin, and Ray Sinnott. 2013a. "Chapter 7 - Capital Cost Estimating." In *Chemical Engineering Design (Second Edition)*, edited by Gavin Towler and Ray Sinnott, 307–54. Boston: Butterworth-Heinemann. https://doi.org/10.1016/B978-0-08-096659-5.00007-9.

Towler, Gavin, and Ray Sinnott. 2013b. "Chapter 8 - Estimating Revenues and Production Costs." In *Chemical Engineering Design (Second Edition)*, edited by Gavin Towler and Ray Sinnott, 355–87. Boston: Butterworth-Heinemann. https://doi.org/10.1016/B978-0-08-096659-5.00008-0.

Turton, Richard, Joseph Shaeiwitz, Debangsu Bhattacharyya, and Wallace Whiting. 2018. *Analysis, Synthesis, and Design of Chemical Processes*. Boston.

UN. 1987. "Report of the World Commission on Environment and Development: Our Common Future." United Nations, New York. https://sustainabledevelopment.un.org/content/documents/5987our-common-future.pdf.

U.S. Department of Energy. 2015. "Hydrogen and Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan." https://www.energy.gov/eere/fuelcells/articles/hydrogen-and-fuel-cell-technologies-office-multi-year-research-development.

Vadlamani, Agasteswar, Jeremy Weir, Xiaofei Zhao, Sridhar Viamajala, and Sasidhar Varanasi. 2014. *Assessment of Temperature- and PH-Sensitive Hydrogels for Dewatering Dilute Algal Suspensions*.

Valente, Antonio, Diego Iribarren, Daniele Candelaresi, Giuseppe Spazzafumo, and Javier Dufour. 2020. "Using Harmonised Life-Cycle Indicators to Explore the Role of Hydrogen in the Environmental Performance of Fuel Cell Electric Vehicles." *International Journal of Hydrogen Energy*, Special Issue on HYPOTHESIS XIV, 45 (47): 25758–65. https://doi.org/10.1016/j.ijhydene.2019.09.059.

Van der Drift, A., H. Boerrigter, B. Coda, M. K. Cieplik, and K. Hemmes. 2004. "Entrained Flow Gasification of Biomass. Ash Behaviour, Feeding Issues, System Analyses," April. https://www.osti.gov/etdeweb/biblio/20479502.

Virtanen, Pauli, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, et al. 2020. "SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python." *Nature Methods* 17: 261–72. https://doi.org/10.1038/s41592-019-0686-2.

Visconti, Carlo Giorgio, and Marina Mascellaro. 2013. "Calculating the Product Yields and the Vapor–Liquid Equilibrium in the Low-Temperature Fischer–Tropsch Synthesis." *Catalysis Today*, Fuels and Chemicals from Synthesis Gas: State of the Art, 214 (October): 61–73. https://doi.org/10.1016/j.cattod.2012.10.016.

Wang, Liming, Fangyi Li, Jianfeng Li, and Xiaowei Wang. 2010. "Sensitivity and Uncertainty Analysis of Life-Cycle Assessment Based on Multivariate Regression Analysis." In *5th International Conference on Responsive Manufacturing - Green Manufacturing (ICRM 2010)*, 184–91. https://doi.org/10.1049/cp.2010.0434.

Wang, Michael, Amgad Elgowainy, Uisung Lee, Adarsh Bafana, Pahola Thathiana Benavides, Andrew Burnham, Hao Cai, et al. 2020. "Summary of Expansions and Updates in GREET® 2020." ANL/ESD-20/9. Argonne National Lab. (ANL), Argonne, IL (United States). https://doi.org/10.2172/1671788.

Wernet, Gregor, Christian Bauer, Bernhard Steubing, Jürgen Reinhard, Emilia Moreno-Ruiz, and Bo Weidema. 2016. "The Ecoinvent Database Version 3 (Part I): Overview and Methodology." *The International Journal of Life Cycle Assessment* 21 (9): 1218–30. https://doi.org/10.1007/s11367-016-1087-8.

Woodward, David G. 1997. "Life Cycle Costing—Theory, Information Acquisition and Application." *International Journal of Project Management* 15 (6): 335–44. https://doi.org/10.1016/S0263-7863(96)00089-0.

Woolcock, Patrick J., and Robert C. Brown. 2013. "A Review of Cleaning Technologies for Biomass-Derived Syngas." *Biomass and Bioenergy* 52 (May): 54–84. https://doi.org/10.1016/j.biombioe.2013.02.036.

World Resources Institute. 2022. "Climate Watch." 2022. https://www.climatewatchdata.org/.

Wu, Wei, Keng-Hsien Lin, and Jo-Shu Chang. 2018. "Economic and Life-Cycle Greenhouse Gas Optimization of Microalgae-to-Biofuels Chains." *Bioresource Technology* 267 (November): 550–59. https://doi.org/10.1016/j.biortech.2018.07.083.

Wunderlich, Johannes, Katy Armstrong, Georg A. Buchner, Peter Styring, and Reinhard Schomäcker. 2021. "Integration of Techno-Economic and Life Cycle Assessment: Defining and Applying Integration Types for Chemical Technology Development." *Journal of Cleaner Production* 287 (March): 125021. https://doi.org/10.1016/j.jclepro.2020.125021.

Zhang, Qingfu, and Hui Li. 2007. "MOEA/D: A Multiobjective Evolutionary Algorithm Based on Decomposition." *IEEE Transactions on Evolutionary Computation* 11 (6): 712–31. https://doi.org/10.1109/TEVC.2007.892759.

Zheng, Guozhong, and Xiao Wang. 2020. "The Comprehensive Evaluation of Renewable Energy System Schemes in Tourist Resorts Based on VIKOR Method." *Energy* 193 (February): 116676. https://doi.org/10.1016/j.energy.2019.116676.

Zhu, Yunhua, Karl O. Albrecht, Douglas C. Elliott, Richard T. Hallen, and Susanne B. Jones. 2013. "Development of Hydrothermal Liquefaction and Upgrading Technologies for Lipid-Extracted Algae Conversion to Liquid Fuels." *Algal Research* 2 (4): 455–64. https://doi.org/10.1016/j.algal.2013.07.003.

Zimmermann, Arno W., Johannes Wunderlich, Leonard Müller, Georg A. Buchner, Annika Marxen, Stavros Michailos, Katy Armstrong, et al. 2020. "Techno-

Economic Assessment Guidelines for CO2 Utilization." *Frontiers in Energy Research* 8. https://www.frontiersin.org/articles/10.3389/fenrg.2020.00005.

Zitzler, Eckart. 2002. "Evolutionary Algorithms for Multiobjective Optimization." *Evolutionary Methods for Design, Optimisation, and Control, CIMNE*, 19–26.

Zitzler, Eckart, and Simon Künzli. 2004. "Indicator-Based Selection in Multiobjective Search." In *Parallel Problem Solving from Nature - PPSN VIII*, edited by Xin Yao, Edmund K. Burke, José A. Lozano, Jim Smith, Juan Julián Merelo-Guervós, John A. Bullinaria, Jonathan E. Rowe, Peter Tiňo, Ata Kabán, and Hans-Paul Schwefel, 832–42. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer. https://doi.org/10.1007/978-3-540-30217-9_84.

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