CEN Workshop Agreement

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Evaluation of Process Intensification of Biorefining Processes for Economic and Sustainability Viability – EvaPIBioref

Bewertung der Prozessintensivierung von Bioraffinerie-Prozessen im Hinblick auf Wirtschaftlichkeit und Nachhaltigkeit - EvaPIBioref

Évaluation de l'intensification des procédés de bioraffinage en vue d'une viabilité économique et durable - EvaPIBioref

CCMC will prepare and attach the official title page.

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European foreword

This CEN Workshop Agreement has been developed in accordance with the CEN-CENELEC Guide 29 “CEN/CENELEC Workshop Agreements – A rapid prototyping to standardization” and with the relevant provisions of CEN/CENELEC Internal Regulations - Part 2. It was approved by a Workshop of representatives of interested parties on YYYY-MM-DD, the constitution of which was supported by CEN following the public call for participation made on 2023-10-05. However, this CEN Workshop Agreement does not necessarily include all relevant stakeholders.

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Introduction

The objective of process intensification (PI) in the context of biorefining operations is to lead to a reduction in operation costs, feedstock and energy resources, greenhouse gas emissions and higher yields, while increasing operation safety, by concentrating on technologies which can intensify processes and create an integrated biorefinery concept. PI strategies in general and specifically for biorefining operations have not featured strongly in the vast standards literature. However, examining the Standards and Guidance Documents prepared or under consideration by the CEN/CENELEC Technical Committees, it is possible to identify a significant number where these innovative processing strategies will impact the bioeconomy from the process, safety, economic and /or environmental aspects.

Bio-based feedstocks encompass a multitude of materials from agricultural and forest residues to industrial and municipal wastes. Lignocellulose is one type of feedstock which emanates from forestry and agricultural waste and constitutes non-edible biomass. Therefore, it is of particular importance for the bioeconomy as the sustainable source of raw materials for the production of bio-based chemicals and materials as well as advanced biofuels. In Europe alone, lignocellulosic biomass has an estimated annual potential of technical availability of 1372 Mt, which could be sustainably used by 2030 [1], doubling the current usage. However, in order to reach the goal of 25 % bio-based chemicals in 2030 (2015: 14 %), a major increase of the usage and processing efficiency of lignocellulosic biomass for sourcing the chemical industry would be required.

Processes are well established to valorise only two of the three major components in lignocellulose, i.e. cellulose (for fibres) and lignin (for energy). Hemicelluloses, which typically account for 20-30 % (w/w), are often not efficiently segregated, purified, converted and transformed into useful and application-ready compounds, and thus are relatively under-exploited. This results in less efficient use of the lignocellulosic raw material and high volume waste fractions, making current products from lignocellulosic biorefineries uneconomical and less sustainable.

In the BioSPRINT project[1], PI is used to produce valuable polymers from hemicelluloses by intensifying four process steps:

1. Upstream purification and concentration of sugars in the hemicelluloses stream
2. Catalytic conversion of the mixed sugar fractions to furans
3. Downstream purification of furan monomers
4. Polymerisation of the monomers to resole and novolac-type resins as well as Mannich polyols

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[1] Biorefining of sugars via Process Intensification. Project under the call Horizon 2020-BBI-2019-SO2-R6, GA Number: 887226; https: https://biosprint-project.eu/

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1 Scope

This CWA provides guidance for evaluating if the use of process intensification measures for biorefining processes is economically and sustainably viable.

The CWA is intended to be used by biorefinery plant manufacturers, its owners and operators as well as process design engineers. Since conventional refining of plant biomass often needs to process diluted aqueous product streams still containing lots of by-products and impurities, energy- and cost-intensive upstream and downstream processes are essential for product recovery. Thus, the aim of this CWA is to provide an evaluation procedure to assess whether PI measures are sustainably and economically meaningful against the conventional processes.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

CWA 17484:2020, *Anaerobic digestion plants — Feasibility assessment methodology for integrating a Volatile Fatty Acid Platform Technology*

ISO/CD TS 14076:2024, *Eco-Technoeconomic Analyses: Principles, requirements and guidelines*

VDI 2776 (E), Blatt 2:2024, *Process engineering plants*

EN ISO 10991:2009, *Micro process engineering*

VDI 4075, Blatt 1:2014-10, *Cleaner production (PIUS)*

VDI 6310 Blatt 1:2016-01, *Classification and quality criteria of biorefineries*

EN 16214-1:2020[2], *Sustainability criteria for the production of biofuels and bioliquids for energy applications - Principles, criteria, indicators and verifiers - Part 1: Terminology*

CEN/TS 16214-2:2020, *Sustainability criteria for the production of biofuels and bioliquids for energy applications - Principles, criteria, indicators and verifiers - Part 2: Conformity assessment including chain of custody and mass balance*

EN 16214-3:2017[3], *Sustainability criteria for the production of biofuels and bioliquids for energy applications - Principles, criteria, indicators and verifiers - Part 3: Biodiversity and environmental aspects related to nature protection purposes*

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[2] As impacted by German version EN 16214-1:2012/A1:2019.

[3] As impacted by German version EN 16214-3:2012/A1:2017.

EN 16214-4:2020, *Sustainability criteria for the production of biofuels and bioliquids for energy applications - Principles, criteria, indicators and verifiers - Part 4: Calculation methods of the greenhouse gas emission balance using a life cycle analysis approach*

EN ISO 14040:2006-07, *Environmental management — Life cycle assessment — Principles and framework*

EN ISO 14044:2006-10, *Environmental management — Life cycle assessment — Requirements and guidelines*

EN ISO 14046:2016-07, *Environmental management — Water footprint — Principles, requirements and guidelines*

EN ISO 14050:2020, *Environmental management — Vocabulary*

EN ISO 14067:2018, *Greenhouse gases – Carbon footprint of products – Requirements and guidelines for quantification*

ISO/DIS 14075:2023, *Environmental management — Principles and framework for social life cycle assessment*

EN 16575:2014, *Bio-based products — Vocabulary*

EN 16760:2015, *Bio-based products — Life Cycle Assessment*

ISO Guide 82:2019, *Guidelines for addressing sustainability in standards*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp/

— IEC Electropedia: available at https://www.electropedia.org/

3.1
Process Intensification

Any chemical engineering development that leads to a substantially smaller, more environmental friendly and energy efficient technology.

3.2
Sustainable development

development that meets the environmental, social and economic needs of the present without compromising the ability of future generations to meet their own needs.

Note 1 to entry: Derived from the Brundtland Report [27]

[SOURCE:ISO Guide 82:2019, 3.2]

3.3

Sustainability

state of the global system, including environmental, social and economic aspects, in which the needs of the present are met without compromising the ability of future generations to meet their own needs.

Note 1 to entry: The environmental, social and economic aspects interact, are interdependent and are often referred to as the three dimensions of sustainability

Note 2 to entry: Sustainability is the goal of sustainable development (3.2).

[SOURCE:ISO Guide 82:2019, 3.1]

3.4

Sustainability assessment

assessment of the contribution of a product to the sustainable development (3.2), based on the results of an environmental, social and economic performance assessment and under the precondition of fulfilment of technical, functional, legal and other requirements.

Note 1 to entry: Environmental, social and economic performance are of equal importance. For new products, the assessment is based on scenario-related calculations; for existing products, the assessment is based partially on actual, measured data.

Note 2 to entry: Sustainability is the goal of sustainable development (3.2).

[SOURCE:ISO 21931-1:2022, 3.5.1, modified to address products instead of buildings]

4 Symbols and abbreviations

AACE	American Association of Cost Engineers
ACR	Agitated Cell Reactor
BioSPRINT	Biorefining of sugars via Process Intensification. Project under the call Horizon 2020-BBI-2019-SO2-R6, GA Number: 887226
C5	Containing five carbon atoms
C6	Containing six carbon atoms
CAPEX	Capital expenditure
CFD	Computational Fluid Dynamics
EN	European Standard
eTEA	Eco-Technoeconomic Analysis
EvaPIBioref	Evaluation of Process Intensification of Biorefining Processes for Economic and Sustainability Viability
FEL	Front-End Loading
gPROMS	general PROcess Modelling System
ILCSA	Integrated Life Cycle Sustainability Assessment
ISO	International Organization for Standardization

LCA	Life cycle assessment
LCC	Life cycle cost
LCI	Life cycle inventory analysis
LCIA	Life cycle impact assessment
MOF	metal-organic framework
Mt	million tonnes
OPEX	Operating expenditure
p	Pressure
PI	Process Intensification
PSILCA	Product Social Impact Life Cycle Assessment
R&D	Research and development
RP	Recommended practice
RTR	Rotating Tube Reactor
S-LCA	Social life cycle assessment
SDR	Spinning Disc Reactor
SHDB	Social Hotspots Database
T	Temperature
TEA	Techno-economic assessment
TS	Technical Standard
UV/Vis	Ultraviolet/Visible

5 Intention and drivers for integrating process intensification in biorefinery context

The role of biorefinery sector in mitigating climate change and achieving net zero in the chemical process industry has become increasingly important over the last decade. The valorisation of bio-based feedstocks into useful building block chemicals serving as replacements for fossil-based counterparts plays a key part in this quest. However, the processing and economic challenges faced by the biorefinery sector have presented significant obstacles in realising the potentials of biorefineries to move away from fossil-based chemicals.

The processing challenges are related to the often complex biomass feed streams such as hemicellulose liquors which, while rich in water, also contain a number of different impurity and inhibitor molecules at low concentrations (e.g short chain acids, extractives, dissolved inorganic compounds and residual lignin among others) alongside the C5 and C6 monomeric and oligomeric sugars. These molecules often complicate the sugar conversion steps and lead to resource-intensive downstream purification steps, thus resulting in low biorefinery yields in general and poor product grade in many cases. To purify such streams traditionally requires multi-step, energy-intensive processes such as evaporation, distillation and crystallisation, with generation of high volumes of wastewater and by-products. Similarly, the catalytic step for the conversion of sugars into platform molecules such as furan-based derivatives suffers from low selectivity due to highly reactive intermediates, which combined with inefficiencies in mixing and heat and mass transfer as well as broad residence times encountered in large scale conventional stirred tank vessels, can react further to undesirable by-products. Many of these processing challenges can be addressed by the consideration and implementation of intensification strategies in the individual process steps and ideally integrated across the whole biorefinery process.

6 Identification and description of the framework to be considered

Process Intensification (PI) is a process design strategy in chemical engineering which involves the development of innovative reaction and separation technologies, processing methods and materials leading to improved performance in mixing, heat and mass transfer for greater productivity. Often, all three dimensions – technologies, methods and materials – are deployed in combination to achieve maximum impact on the process (see Figure 1- showing overlaps between technology, methods and material).

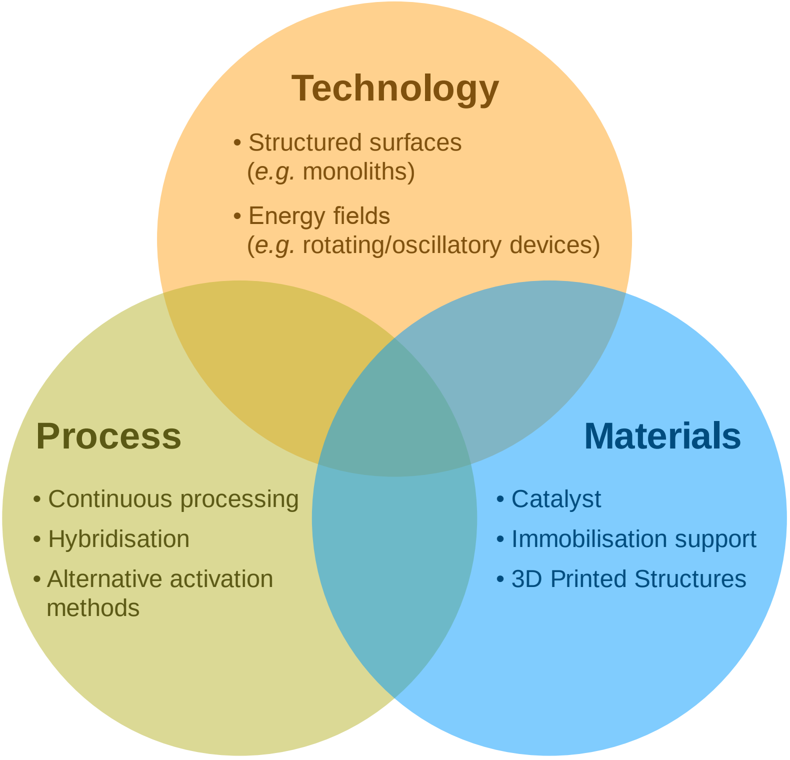

Figure 1 Process intensification innovation toolbox

6.1 Drivers for process intensification

PI philosophy is based on the substitution of traditional unit operations with more innovative, efficient technologies and processing methods, often leading to significant reductions in processing equipment volume (at least 1 to 2 orders of magnitude reduction in scale ideally [2]). At the molecular level, bringing molecules in closer proximity in compact devices with larger surface areas means mixing and heat and mass transfer limitations can be overcome for inherent reaction and separation rates to prevail. Reduced energy consumption, waste formation and safety risks of hazardous materials are some of the benefits of such reductions in scale which result in greater process efficiency and environmental sustainability. At the plant level, the realisation of miniaturised, modular plants opens up the opportunity for decentralisation of the supply chain, contributing to economic viability of the business. Figure 2 summarises the main benefits of the PI strategy (adapted from [3]).

It is to be noted that there is a distinction to be made between process intensification and process optimisation where the former involves a step change in methodology and efficiency while the latter pursues incremental and therefore more limited changes [4]. Once an intensified processing solution is identified, optimisation is still possible by adjusting process parameters such as temperature, pressure, flowrates and/or a technology-specific active enhancement parameter (e.g., speed of surface or packed bed rotation, light intensity for light-driven transformations).

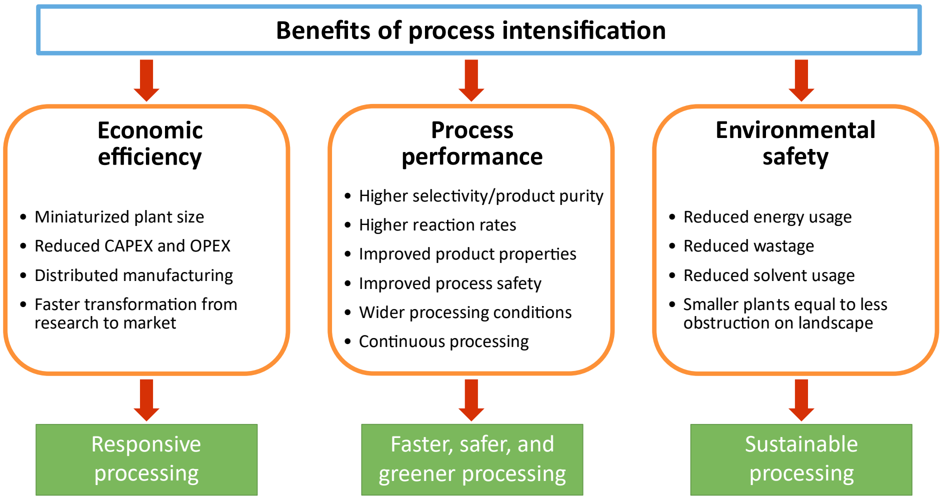

Figure 2 Economic, process, and environmental benefits of process intensification (Adapted from [3])

6.2 Process intensification options

6.2.1 Introduction

As indicated above, process intensification options can entail technology, processes, materials or a combination of these. The information in the sections that follow can be used to identify examples of commonly useful intensification concepts to address key process limitations and guide the reader in choosing appropriate process intensification strategies with potential to enhance the process. This information can also be used to guide further research for additional intensification strategies in specialised textbooks, journal articles and industrial expos, all of which is encouraged. A few examples of less commonly used technology are also illustrated to demonstrate the possibility to exploit further intensification effects where demanding applications are encountered, and where through engineering creativity and innovation one was able to find more bespoke solutions.

The classification between technology/equipment, processes/methods and materials is not watertight. As shown in Figure 1, there are overlaps between these. For example, compact heat exchangers, microchannels and monolith equipment often rely on materials development, and some of the examples in Table 1 rely on continuous processes, or can be used with combined with alternative activation methods. Where required, a combined use of multiple strategies is often encountered to maximise the benefits of intensification.

6.2.2 Process intensification equipment

Process intensification can be achieved by innovations in terms of the types of equipment used to carry out different process steps, such as mixing, heating/cooling, reactions or separations. Table 1 below contains a non-exhaustive list of intensified process equipment, with well-established technologies in the field and their principles of operation, indication of the process steps limiting the rate or equilibrium and that are therefore targeted for intensification, generic applications and limitations.

Table 1 Examples of process intensification equipment and technologies

Equipment	Intensification Principle(s)	Target Limiting Step	Applications	Limitations
Static Mixer	Internal pipe structures disrupt flow and induce passive mixing.	Momentum transfer.	Various inline mixing applications.	Not suitable for streams with very coarse particles.
Compact Heat Exchangers	Reduction of diffusion path. Maximisation of surface area.	Heat Transfer.	Gas-gas heat transfer.	Not suitable for processes with solids or fouling fluids.
Microchannels	Reduction of diffusion path.	Heat and/or mass transfer.	Heat transfer, liquid-liquid extraction or reactions, gas-liquid reactions, very endo/exothermic reactions.	Difficult use in processes with solids or fouling fluids. Pressure drop can be high if long residence times and/or long channels are required, and/or very viscous fluids are used.
Monolith Reactor	Reduction of diffusion path. Maximisation of surface area.	Mass transfer.	Catalytic reactions with immobilised catalyst.	Not suitable for streams with very coarse particles.
Coil reactor	The curvature of the reactor channels induces secondary flows through Dean vortices, promoting passive radial flow.	Heat and/or mass transfer.	Various reactions, precipitation or crystallisation processes suitable for plug flow operation, where heat and/or mass transfer between the fluid and the reactor walls limit the process rate, or where slurries with small particles are flow requiring gentle mixing to prevent settling.	
Agitated Cell Reactor	Recreation of a cascade of continuous stirred tanks effect using a single reactor through agitation of a reactor block with multiple cells and agitators.	Heat and/or mass transfer.	Heat and/or mass transfer limited processes that benefit from staged operation or plug flow, *e.g*. multiphase reactions with kinetics suited for plug flow/tubular reactors, or liquid-liquid extraction. Slow processes where	More suitable for fine to speciality chemical applications as larger process scales may require numbering up where a cascade of continuous stirred tank reactors may be more cost effective. Process development and scale

			decoupling between mixing and residence time is required.	will still be more cost effective using the intensified reactor technology though.
Oscillatory Baffled Reactor	Recreation of a cascade of continuous stirred tanks effect through superimposition of a fluid flow oscillation on the net flow direction within a single tubular reactor with multiple internal baffles and cells.	Heat and/or mass transfer.	Heat and/or mass transfer limited processes that benefit from staged operation or plug flow, *e.g.*, multiphase reactions with kinetics suited for plug flow/tubular reactors, or liquid-liquid extraction. Slow processes where decoupling between mixing and residence time is required.	More suitable for fine to speciality chemical applications as larger process scales may require numbering up where a cascade of continuous stirred tank reactors may be more cost effective. Process development and scale will still be more cost effective using the intensified reactor technology though.
Spinning Disc	Mixing enhancement through centrifugal force field. Thin films.	Heat and mass transfer; intraphase mixing	Inherently fast, exo- or endothermic reactions, evaporation and separation. Processes requiring rapid mixing, *e.g.* crystallisation, precipitation	Not always suitable for processes with slow intrinsic kinetics.
Rotating Packed Bed	Mixing enhancement through centrifugal force field. Thin films.	Mass transfer	Rapid interphase mixing, *e.g.* gaseous absorption/desorption, liquid-liquid extraction, distillation.	Not always suitable for processes with slow intrinsic kinetics.
Centrifugal Devices	Mixing or separation enhancement through centrifugal force field. Thin films.	Momentum and/or Mass transfer	Separation of phases in solid-liquid or liquid-liquid multiphase systems. Biphasic liquid-liquid extraction and/or reactions where not only high shear is required to enhance the mass transfer rate, but a large interfacial contact area is also necessary.	
Jet-Impingement Reactor	Jets of reactant flows are created by pressurising the streams and forcing them through an orifice or slit. By impinging the jets into	Momentum and/or heating and/or mass transfer	Cooling applications where fluid amount if limited or there is a high cost. Liquid phase reactions where fast mixing of reagents is required.	

	each other or onto a surface, complete mixing and large contact areas are generated.			

6.2.3 Process intensification methods

Process intensification can also be achieved through innovation in the methods or processes employed, such as hybridisation of reaction and separation process steps into a single piece of equipment, energy integration of multiple steps to reuse energy across a chain of steps, use of alternative activation methods, or use of period operation regimes. Table 2 below contains a non-exhaustive list of intensification methods, with well-established processes in the field and their principles of operation, indication of the process steps limiting the rate or equilibrium and which are therefore targeted for intensification, generic applications and limitations

Table 2 Examples of process intensification methods and processes

Method	**Intensification Principle(s)**	**Target Limiting Step**	**Applications**	**Limitations**
Mechanical Vapour Recompression	Heat integration technique in which a vapour is mechanically compressed, with resulting increase in temperature. The compressed vapour is then used to heat a process fluid elsewhere in the process to a temperature above what would normally be possible with just simple heat exchanged without recompression.	Energy consumption.	Distillation and evaporation where the vapour exiting the unit is recompressed and used to reboil the liquid at the bottom of the unit.	
Reactive Distillation	Integration of reaction and distillation in a single unit. Reaction can be used to drive the separation (*e.g.* overcoming azeotropes or displacing equilibrium), or the separation can be used to drive the reactions (*e.g.* displacement of reaction equilibrium or eliminations of catalyst inhibitors).	Mass transfer and/or chemical/physical equilibrium.	Reduction in equipment footprint and capital costs by combining reaction and separation in a single unit. Purification of streams where vapour-liquid equilibrium is limiting and conversion of some of the species in the reaction step will displace physical equilibrium. Increase in reaction conversion in equilibrium-limited reactions when removal of the reaction products is beneficial for displacement of chemical equilibrium, or when catalyst inhibitor species form and required removal.	Reaction and distillation must share common windows for operating conditions. Products and side-products boiling points need to appropriately align in sequence of separation.
Reactive Extraction	Chemical reaction is used to displace solubility equilibrium.	Solubility equilibrium.	Systems where the species of interest has a low solubility in the extraction solvent, and where a subsequent reaction is necessary and can used to	

			displace the solubility equilibrium, or where the extracted component can be converted to leave a clean matrix in the solid phase. Systems where the extraction solvent is costly and reaction can aid in increasing the extraction capacity of the solvent.	
Extractive Reaction	Extraction is used to displace reaction equilibrium.	Chemical equilibrium.	Systems where the reaction conversion is limited by chemical equilibrium, and the products can be separated by liquid-liquid extraction. Systems where the reaction product is a reactive intermedia unstable in the reaction medium, or where catalyst inhibitors are produced during the reaction requiring immediate separation.	
Membrane Reactors	Hybridisation process combining membrane separation with chemical reaction. A membrane is coated/embed with catalyst and used to catalyse the reaction with simultaneous separation of reaction products/side products/reactive intermediates, preventing further reaction/decomposition and/or displacing chemical equilibrium and/or increasing driving force for membrane filtration (if reaction carried out on the filtrate side). Increase in	Mass transfer and/or chemical/physical equilibrium.	Reduction in equipment footprint and capital costs by combining reaction and separation in a single unit. Purification of streams where membrane filtration rates are limiting and conversion of the species in the filtration will accelerate the filtration rate. Increase in reaction conversion in equilibrium-limited reactions when removal of the reaction products is beneficial for displacement of chemical equilibrium. Isolation and stabilisation of reaction products where those are reactive intermediates. Increase in reaction rates in multiphase gas-liquid-solid	Processes where fouling occurs can required regular membrane cleaning cycles or membrane replacement.

	contact surface area between catalyst and fluids.		systems where a high interfacial area is required (*e.g.* fuel cells).	
Membrane Distillation	Separation of chemical species based on permeability characteristics of a vapour through a membrane, whilst retaining the liquid.	Vapour-liquid equilibrium and/or energy consumption.	Systems where only water vapour is required to permeate, although systems also exist for other separations, *e.g.* ethanol removal.	Can have a higher energy consumption then other more conventional membrane filtration options.
Partition Wall Column	Thermal and mechanical integration of multiple distillation columns into a single column. A vertical partition inside the column is used to divide the feed zone and the product draw, preventing remixing and allowing heat integration between the rectification and stripping zones.	Energy consumption.	Reduction of capital and operating costs, and greenhouse gas emissions, in complex distillation operations requiring multiple columns operating at similar pressures, and where energy integration between rectifying and stripping sections in different separation units can be integrated into a single column through the use of dividing partitions.	
Ultrasound	Ultrasound waves generate microscopic cavitation centres, which upon collapse of the gas bubbles release localised energy.	Momentum and/or Heat transfer.		
Light	Use of electromagnetic radiation in the UV/Vis region of the spectrum to active a process.	Alternative activation method.	Reactions where UV/Vis light can excite and activate reactants. Photocatalytic processes where a catalyst is activated by UV/Vis radiation.	
Microwaves	Volumetric heating using electromagnetic radiation in the	Heat transfer.	Processes where uniform heating is required and where it is difficult to	Materials need to have a dipole moment in order to interact with the microwaves.

	microwave region of the spectrum to active a process.		carry out mixing, *e.g.* solid/very viscous phases, ceramics drying, etc.	
Plasma	A strong electrical field causes a gas to ionise and conduct electricity.	Alternative activation method.	Systems where radical chemistries can accelerate or allow reactions to progress through alternative pathways faster or not accessible to conventional thermal activation methods.	
Periodic Operation	Periodic oscillations in operating conditions (particularly in flow rate) destabilise steady state operation and disrupt boundary layers, enhancing transport rates.	Heat and/or mass transfer.	Gas-liquid-solid reactions (i.e. trickle bed reactors) where a solid catalyst is used, and the gas is mostly insoluble in the liquid phase benefit from periodic oscillation of gas and liquid flows to enhance adsorption of all species onto the catalyst surface. Fuel cells with diffusion limited reactions benefit from oscillatory flows to disrupt boundar layers and increase mass transport rates.	

6.2.4 Process intensification materials

Process intensification can also be achieved through innovation in the materials used, which can influence how catalytic reactions occur, condition mass transfer, promote heat transfer, or even influence mixing. Table 3 below contains examples of intensification through materials strategies. Although a more recent concept than conventional intensification through technology/equipment or processes/methods, there are some well-established materials in the field that can achieve significant process enhancements.

Table 3 Examples of process intensification materials.

Material	**Intensification Principle(s)**	**Target Limiting Step**	**Applications**	**Limitations**
Catalysts (*e.g.* Zeolites, MOFs,	Molecular structure selectivity, selective permeability, controlled wettability, responsiveness to microwaves or induction heating.	Chemical reaction, mass transfer, heat transfer.	Diverse catalytic reactions where selectivity control is crucial or difficult to achieve through conventional catalysis methods, or where transport limitations within the catalyst are required, or where electrification of process heating is desirable. Use of immobilised catalysts is desirable for an integrated reaction-catalyst separation step; this may require development of heterogeneous catalysts and immobilisation strategies compatible with the process under consideration	Both the material properties that enhance selectivity or transport rates and the catalyst activity are related to the catalyst chemical composition and structure. It is not always possible to find suitable materials that address the limitations and can be catalytically active. Catalyst immobilisation in e.g. fixed bed reactors may introduce mass transfer limitations.
Solvents (*e.g.* ionic liquids)	Control of intermolecular interactions with promotion or suppression of specific reactions.	Chemical reaction and/or mass transfer.	Diverse chemical reactions.	
Porous materials	Molecular structure selectivity, porosity/capillary action, responsiveness to magnetic field.	Mass transfer.	Mass transfer intensification in separation processes such as distillation, extraction, or membrane filtration, amongst others.	
Membranes	Polymeric or ceramic membranes where separation selectivity is driven by molecular shape, and/or size, and/or chemical properties (*e.g.* polarity). Liquid membranes	Mass transfer.	Chemical separation/purification processes, particularly where separation is possible based on molecular shape/size/selective diffusion through a medium. Often driven by desire to avoid thermal	Processes with large amounts of solids of streams prone to fouling may require frequent membrane backwashing or replacement.

	where a liquid solution is lodged into a porous membrane scaffold, with the liquid controlling the separation selectivity.		composition or additional solvent consumption.	
Thermally Conductive Materials	Structured materials with enhanced thermal conductivity.	Heat transfer	Use of structured packing, foams or nanoparticles to enhance heat flows in packed bed reactors and prevent reaction runaway, general heat transfer.	
Magnetic Materials	Retention of solid particles in a magnetic field. Cooling in magnetocaloric materials through cycling magnetisation and demagnetisation.	Mass transfer, heat transfer.	Recovery and reuse of catalysts or heat transfer aids. Cooling.	
Controlled wettability materials	Increase in heat flux during nucleate boiling in super-hydrophilic surfaces. Control of dropwise condensation using super-hydrophobic surfaces. Reduction of drag.	Heat transfer, momentum transfer.	Boiling and condensation systems, reboilers, condensers, evaporators.	Chemical compatibility with the surface materials is required.
Polymers and surfactant additives	Reduction in drag in flow through modification of the boundary layer phenomena.	Momentum transfer.	Increase in flow in difficult streams, reduction in pumping costs.	Additives must not cause an issue in terms of stream purity.

6.3 Training/Education

Process intensification has been a rapidly growing field in recent decades, aiming to maximize process efficiency by reducing the number of steps or equipment, focusing on more efficient heat and mass transfer, and integrating new approaches to downstream and upstream separations. Despite the numerous benefits and the direct impact on process safety, energy efficiency and cleaner processing, PI as a new, emerging field is often met with scepticism due to a lack of awareness and technical knowledge of such process development strategies. Therefore, proper training and education programmes are one of the most important aspects when it comes to the dissemination of process intensification as an engineering tool for improving processes, especially in the biorefinery sector, to overcome possible concerns due to the diverse perspectives of different professional groups.

In recent years, a number of degree programmes around the world, mostly focused on chemical engineering, have incorporated elements of process intensification in taught courses to undergraduate and post-graduate students [5]. However, there is scope to adapt these engineering focused courses to wider science-based programmes so that the fundamentals of process intensification can be integrated within curricula of higher education for various professions such as chemists, chemical engineers and other majors in natural sciences in order to facilitate the understanding, acceptance and implementation of new technologies. These courses should be underpinned by problem- or challenge-based learning of PI techniques, as highlighted in several documented examples in [6].

Alongside developing awareness and knowledge of PI via education programmes, it is also important to actively disseminate knowledge and train the experts already working in related fields such as chemists, chemical engineers, bioprocessing engineers etc. It is important to approach the implementation of PI comprehensively not only in academia but also in various sectors linked to chemical, fine chemicals, pharmaceutical industries amongst many others. Therefore, it is of great importance to educate the personnel at the operational level of the plans about PI techniques and to familiarize the process operators with the required protocols. In addition, it is important to clearly present the benefits of PI technologies to policy makers in order to bridge the gap between academia and industry. Great emphasis should also be given to specific skills related to digitization, modelling and data management.

7 Assessment methodology

7.1 Introduction

Evaluation of PI process is based on their feasibility to the problem in hand. First, the potential PI solutions (involving a combination of technology, processing methods and materials) need to be identified and screened (see Section 7.2). The evaluation continues by formulating the necessary models of the intensified process, as indicated in Section 7.3, to create the necessary data to the sustainability assessment (Section 7.4).

It is important to notice that usually the aim is not to perform an isolated assessment of the investigated product system, but to compare the performance to a carefully selected benchmark process to create a baseline for evaluation. Thus, the assessment methodology needs to be repeated for the benchmark case(s), as well. There, the selection of benchmark can be challenging, and several approaches can be taken, such as product-driven (fossil-based counterpart), or process-driven (conventional technologies) comparison.

7.2 Process intensification assessment: a methodological framework

The step-by-step methodology for conducting a PI assessment of a biorefinery process is shown in Figure 3. This follows similar methodologies presented for generic applications [7] and for pharmaceutical [8] and fine chemical processes [9].

A fundamental knowledge-base of the process under consideration is essential in understanding the limitations inherent in the key processing steps leading to the final product. This may require lab testing and process simulation in the early stages to build this knowledge. Matching the ideal process requirements to the engineering capability of technologies, methods and materials in the PI toolbox, examples of which have been highlighted in Section 6.2, is another important stage of this methodology framework. Evaluating the potential of these possible matches for performance enhancement vs. an established, well-defined benchmark depends on laboratory trials supported by modelling and simulation of the novel technologies.

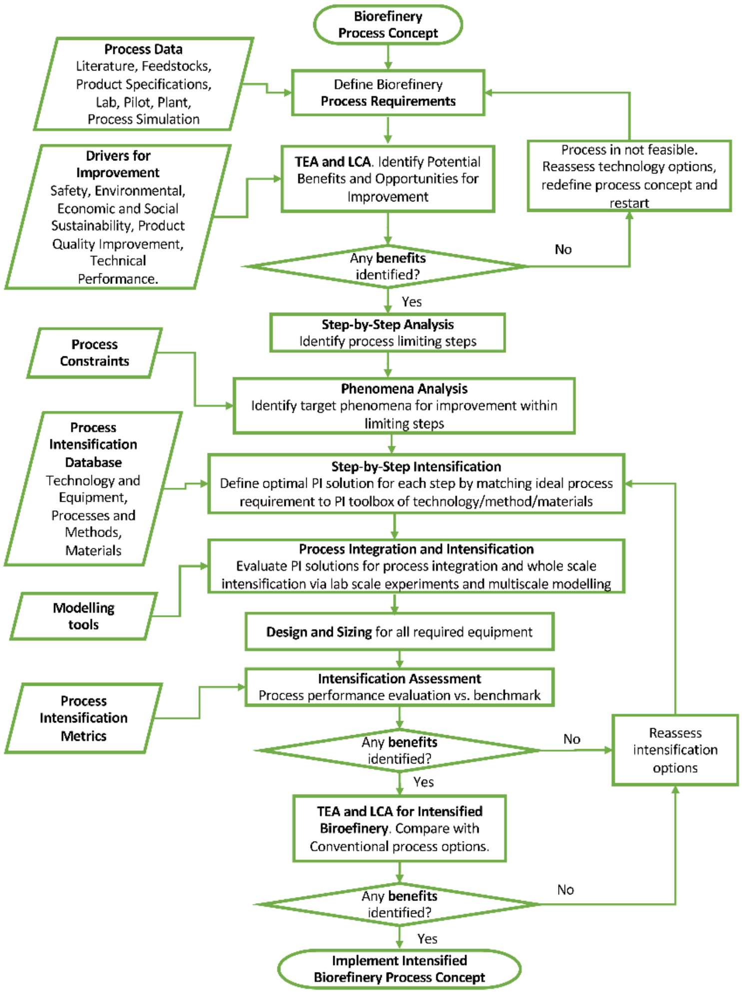

Figure 3 A step-by-step methodology for PI assessment in a biorefinery context (adapted from [8])

7.3 Modelling and simulation

7.3.1 Introduction

Process modelling and simulation are essential tools for evaluating the feasibility of new process concepts. Simulation models can identify technology limitations, risks, and improvement opportunities early on and help researchers focus on areas that matter for achieving technologically and economically viable processes. Model-derived mass and energy balances represent the basis for assessing a commercial process's techno-economic viability, which is crucial for future investment decisions.

Many software tools, available in the market, can perform steady state and dynamic simulation of process systems. Specialised model-based design and optimisation tools often have pre-made modules of the technological processes and unit operations represented in software. However, the user still needs to make modelling decisions and understand the uncertainties related to the simulation results.

7.3.2 System boundaries and scope

The first step in developing simulations is defining boundaries and describing the model's scope. The boundaries are set around the process or the system to be simulated. Mass and energy flows crossing these boundaries represent the model's inputs and outputs. The model's level of detail is typically defined by its purpose and the available budget. For feasibility studies, simulation models usually consider the main unit operation to calculate mass and energy balances. Small and auxiliary equipment is often not considered at the early development stage due to many unknowns surrounding the design and configuration of the process, and they are also unlikely to make a significant difference in performance analysis and the overall economic evaluation More detailed simulation models could provide more accurate insights into the plant design and more comprehensive mass and energy balances; however, more time and effort are needed to build and run such models. Therefore, model purpose versus effort trade-off should be carefully considered, especially in the early stages of process development.

7.3.3 Mass and energy balance

Simulation models are used to calculate mass and energy balances and analyse processes under different operating conditions, capacities and design configurations. Mass and energy balances are basis for designing and sizing process equipment, techno-economic evaluation and lifecycle assessment. The development of mass and energy balances requires: (1) Identification of system boundaries and the components included in the model, (2) development of a process flow diagram for the process units, streams connecting the units and the direction of flows, (3) writing the mass and energy balance equations for each component in the system. Typically, the commercial flowsheet simulators automatically determine the balance equations when the user develops the process flowsheet from the pre-made process unit models.

7.3.4 Data acquisition

7.3.4.1 Introduction

The quality of data and the choice of thermodynamic property models significantly impact the quality of the simulation results, i.e. calculated mass and energy balances. Most commercially available simulators, such as Aspen Plus, Aspen HYSYS, gPROMS, ChemCAD, etc., have extensive databases of pure component's physical properties data and built-in thermodynamic property model packages for predicting the properties for mixtures of two or more chemical components at various process conditions (temperatures and pressures). Property packages are generally divided based on the approach thermodynamic properties, such as the Equation of State, Activity Coefficients and Special Models (e.g. steam tables). These calculations allow the simulation of complex unit operations such as distillation columns, reactors, separators, etc. The choice of the thermodynamic property model depends on the nature and composition of components (e.g. gases, liquids, electrolytes, polar or nonpolar, etc.), operating conditions (temperature and pressures) and the availability of parameters. The guidelines for choosing the thermodynamic property models are widely reported in the literature and often available within commercial simulators as property package wizards.

Vapor-liquid or liquid-liquid equilibrium data or any other physical property of chemical mixtures measured in the laboratory can be used to estimate the parameters of the chosen thermodynamic property models and improve the accuracy of simulation results. Most commercial simulators can use laboratory data for estimating thermodynamic parameters and use them for the simulation models.

Regarding the unit models and models for auxiliary equipment, the commercial software typically provides a library of pre-defined models, where the user can select the preferred models. For PI processing units, the software packages may have limited availability and custom-built models are often needed (see Section 7.3.3.1), indicating further need for data acquisition.

The simulation involves some level uncertainty or partial information in the input data due to analytical uncertainties of compositions, model parameters estimated based on laboratory data, utilization of synthetic streams in experimental characterization of the system, modelling assumption etc. Thus, handling of uncertainties is an important topic and discussed in Section 7.3.3.2.

7.3.4.2 PI process models

PI processes are often non-mature technologies with limited or non-existent descriptions in the simulation software. Thus, involvement of PI equipment in mass and energy balances may require additional manual modelling work. In some cases, two or more simulation blocks are needed to model a single PI equipment where multiple operations occur, e.g. solids precipitation, separation and liquid evaporation. The approach to simulating PI equipment will depend on the available laboratory data and the capability of the simulator to use it in the available simulation blocks or modules. Test data from PI equipment of laboratory or pilot scale should be used to validate the simulation model.

7.3.4.3 Handling of uncertainties

To establish more reliable interpretation of the simulation results, and finally, decision-making, identifying and understanding the sources of uncertainty (physical variability, data uncertainty and modelling errors) is crucial. The model calibration and validation are essential steps of model development. Sensitivity analysis can be extended from design variables into the model inputs and parameters that are affected by the uncertainty sources. Statistical methods, Monte Carlo simulation and robust optimization can be applied to quantify and minimize the impact of uncertainties. Uncertainty in chemical process systems engineering is further discussed e.g. in [10].

7.3.5 Simulation of Upscaling

In order to evaluate the process performance of the industrial-scale system and to provide data to techno-economic assessment (TEA) and life cycle assessment (LCA), the upscaling strategies need to be defined. Whilst conventional processes are more often scaled with respect to size/volume, the PI may require numbering-up the processing units to preserve the PI advantages in mass and heat transfer. Also, the energy integration and material recycling possibilities should be considered in this phase [11].

Regarding the PI equipment, an important challenge related to the simulation of upscaling is that the current data might only show the scalability of the PI up to a certain size. This poses uncertainties to the TEA and LCA. To overcome technological and technical challenges as mentioned, further data acquisition has to be carried out. This will most likely involve laboratory experiments and/or detailed modelling and simulations, such as computational fluid dynamics (CFD). Also, the equipment manufacturer will play a vital role here to supply more in-depth know-how of the equipment and information about the materials used in the construction.

7.4 Sustainability assessment

7.4.1 Introduction

Applying the concept of sustainability to process intensification includes a holistic approach, bringing together the global concerns and goals of sustainable development and the demands and requirements in terms of product functionality, efficiency and economy. Different target audiences have different perspectives on these challenges and the preferred solutions.

There are different methods of sustainability assessment depending on the studied subject; the most common subject is products (any good or service). There are no definitive methods for measuring sustainability or confirming its accomplishment. Quantifying sustainability is typically based on a set of indicators that consider the environmental, social and economic dimension of sustainability. The sustainability performance of a product is usually evaluated based on a relative assessment, i.e. in comparison to another product. This could for example be a comparison of an innovative bio-based product with a conventional fossil-based product. Recently, also absolute sustainability assessments are increasingly performed, especially regarding the environmental dimension. Those involve a comparison to an external list of environmental carrying capacities such as the 1.5 degree climate goal of the Paris Agreement [12] or the Planetary Boundaries concept [13]; [14]; [15]; [16]).

When focussing on products, sustainability assessments evaluate the contribution of that product to sustainable development, based on the results of an environmental, social and economic performance assessment and under the precondition of fulfilment of technical, functional, legal and other requirements. Life-cycle-based approaches play an increasingly significant role for setting performance criteria within methods of assessment of environmental, social and economic performance of products. Three methods for assessing these three classic dimensions (or pillars) of sustainability are presented in the following sections, before moving on to a method for combining LCA, TEA and S-LCA into an integrated sustainability assessment.

7.4.2 Life cycle assessment (LCA)

Life cycle assessment addresses the environmental aspects and potential environmental impacts (e.g., use of resources and the environmental consequences of releases) throughout a product's life cycle from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal (i.e., cradle-to-grave assessment).

EN ISO 14040 and EN ISO 14044 provide the principles & framework as well as the requirements & guidelines for life cycle assessment. This framework is intentionally broad:

- applicable to any product (good or service)
- various questions can be answered (including scenario-based ones)

As a consequence of this broad framework, the individual LCA practitioner has to make a number of decisions, including the definition of settings (e.g., system boundaries, functional unit, data reference) and the selection of impact categories, methods and databases. Since this sometimes limits the comparability of LCA studies, transparency and reproducibility are key. To address these challenges, more specific provisions for selected product categories (e.g., EN 15804 for construction products, EN 16214 for biofuels and bioliquids for energy applications or EN 16760 for bio-based products) and impact categories (e.g., EN ISO 14046 on water footprint or EN ISO 14067 on carbon footprint of products) have been developed over the years.

Nevertheless, LCA is generally recognised as a robust assessment tool with a high depth of application. Of all sustainability-related assessment methods, LCA is considered to be the most advanced. LCA studies comprise four phases (goal and scope definition, inventory analysis, impact assessment, and interpretation). Usually, LCA studies are comparative studies, i.e., two or more products are compared to each other.

The intention of this section is therefore not to “re-invent the wheel” in terms of LCA but to point out important issues that are specifically relevant when performing an LCA study for products obtained via process-intensified manufacturing.

The main challenges include:

- Taking a life cycle perspective: it is essential to evaluate the environmental aspects related to process intensification measures throughout the entire life cycle (of a product or product portfolio) and not just at the level of individual processes

- Establishing a baseline (“reference”, “business-as-usual”, “current scenario”, “counterfactual scenario”, “conventional scenario”, “status quo“) against which the investigated process intensification is compared / benchmarked, especially if no established process exists.
- Accounting for the ongoing transformation towards a green, digital and resilient economy: process concepts developed today should be compatible with a world in the year 2050 that ideally stays within the safe operating space of humanity (“2050-compatible”) in order to avoid exceedance of planetary boundaries but also stranded investments. In this regard, LCA studies should include forward-looking/future scenarios (prospective LCA), which take into account not only changes in the so-called foreground system but also changes in the background system (electricity generation, steel production, etc.)

Currently, a technical standard on Eco-Technoeconomic Analysis (eTEA) is being developed (ISO/WD TS 14076). It aims at combining a techno-economic analysis (TEA) and a life cycle assessment (LCA) in a common framework. Social impacts, however, are typically outside the scope of an eTEA

7.4.3 Techno-economic analysis (TEA)

7.4.3.1 Introduction

Main focus in this section will be on specific items from the BioSPRINT project. The process of scope building will be described in general (high level) with a reference to existing best practices for estimating and financial analysis. Special attention will be directed towards challenges forthcoming from technology and technical matters related to scaling up from laboratory to commercial size operations. This will lead to both risks but also opportunities for future work.

The Association for the Advancement of Cost Engineering (AACE International) has published a series of Recommended Practices (RPs) that are internationally recognized and used by large engineering and owner-operated companies. The published methods and best practices are continuously updated and are related to CAPEX and OPEX that can be very helpful for scoping, estimating, risk analysis and techno-economic analysis. For generic use there are numerous checklist and publications available. Also be aware that commercial companies have their own financial analysis guidelines and accounting rules that will dictate economic analysis and even partly estimating (for example company policy how to deal with spares, depreciation rules, building interest, foreign exchange rates, taxes, etc). Therefore, in this chapter the focus will be on generic scope building and more specifically challenges that are encountered and dealt with for biorefinery projects like BioSPRINT.

7.4.3.2 Definition of the goal of the techno-economic analysis

7.4.3.2.1 Introduction

The first step in the process is a vital one and often not well thought of: the purpose or goal of the techno-economic analysis, hence capital cost estimate and consequential economic analysis. It doesn’t only determine the required accuracy but also the required effort that has to be done. It makes no sense preparing a detailed estimate when for example the scope is preliminary or in a research phase. This would only be more costly, take more time and deliver results that are most likely misleading in terms of accuracy / reliability.

This goal also determines the required/desired accuracy depending on the development stage of the process / project (e.g., research feasibility, conceptual study, basic engineering study). because this also is decisive for the scope that has to be available or be generated. We will focus primarily on the estimating effort since the other economics are directly related to this, similar challenges. In short, in order to prepare an estimate, it is important to understand what stage of process / project development is currently underway, and therefore what scope is or can be available.

Mentioned AACE guidelines also contain an estimate input checklist / maturity matrix. This matrix provides basically the needed input given a certain desired level of estimate (read also accuracy / reliability). The Recommended practices 17R-97 [17] and 18R-97 [18] are introducing cost estimate classification systems, which provide guidelines for applying general principles of estimate classification for capital investment, excluding operating and life-cycle evaluations. Important to notice is that this systematic approach maps phases and stages of estimating combined with a generic maturity and quality matrix. Furthermore, it's applicable to a wide variety of industries. It is recommended to use these RPs to get an early understanding of the needs related to a desired output.

In BioSPRINT's case the starting points are mass and energy balances derived from simulations. These simulations have been prepared with the AspenONE Engineering suite. This set of expert software contains amongst others Aspen Plus family, Aspen Exchanger Design & Rating and Aspen Economic Evaluation. The software offers the possibility of interactive dimensioning from Aspen Plus to Aspen Economics. Within Aspen this process is called 'MAPPING' and can be semi-automated for any regular equipment, like heat exchangers, columns, pumps, vessels, tanks, etc., which are already defined.

There are however, depending on type of project and mass streams and properties, a few catches that need to be reviewed by experts. This is especially the case when new and unproven technologies (like in the BioSPRINT project) are investigated:

- Not all items in the simulation need to be mapped; some items are in the simulation purely for process reasons such as creating a certain pressure by means of a compressor. In a 'real' project however this pressure might be there because for example the stream is delivered to the process from 'outside'
- Materials of construction have to be chosen manually; by default everything is carbon steel
- Equipment needs to be reviewed, especially larger equipment if the sizing is acceptable or has to be adapted.
- Equipment that isn't predefined in the software, such as membrane systems, SDR and ACR/RTR have to be created manually.
- Non-process equipment such as process control, power supply, civil and structures, piping have to be reviewed and also tweaked to fit the project's reality

7.4.3.2.2 Scaling of novel, intensified equipment

As a basis, the mass and energy balance provides the necessary properties (such as temperature, pressure and physical state), flows, as well as chemical compositions. If the Aspen economic software does not have items available representing the equipment, search for similar items or consider if the equipment can be made up of different available items.

Production capacities in intensified process technologies can be increased in two ways, depending on the technology under consideration:

- Scale out: Fixed size equipment like membrane systems, microreactors etc. where size increases may negate the benefits of processing at smaller scales can simply be replicated in parallel to account for the higher throughput required.
- Scale up: Some equipment can be increased in size or scaled up until a certain size is reached that can be feasibly and practically implemented to gather process performance data and operational information. Beyond this practical size, replication of units may still be needed. Take for instance the Agitated Cell Reactor (ACR) used in the BioSPRINT project on a lab scale. The equipment manufacturer offers different scale reactors that are technologically similar. In the case of BioSPRINT the largest possible size available from the manufacturer has been applied and based on simulated flow and residence time the number of parallel units has been derived. Since the

simulations in this case show a high sensitivity between process conditions and residence time (read number of parallel units!) this is a major point of concern, risk or challenge.

- To overcome technological and technical challenges as mentioned, further evaluations are recommended. This will most likely, as in the case of ACR, be laboratory tests combined with CFD modeling and simulations. Also, the equipment manufacturer will play a vital role in this to supply more in-depth know-how of the equipment (for example to assist with CFD modeling) and to recommend material of construction since the simulated process conditions (p and T) at estimated residence time may differ from tested conditions at smaller scale in a laboratory environment but also differ from product specifications as given by manufacturer. It is important to note that these conditions are assumed to be met in reality on a larger scale but could pose a substantial risk to the economic evaluation in the absence of more reliable data.

After completing all items from the scope, it is advised to run a basic check to uncover abnormalities and scope completeness. To do this, first of all the estimator's experience is important and comparisons with similar projects can be of aid. Consider using metrics and historical data, as well as commercially available databases such as Richardson's International Construction Factors: Location Cost Manual [19] and Compass International Construction Cost Estimating Data [20]. If possible, include quotations from equipment vendors.

In the project team, often the estimator is 'a spider in the web' since to have a complete scope all disciplines are an integral part, equipment, piping, civil, steel, process control, electrical, engineering, construction supervision, transport, etc. Also, interactions between these are important to check, for example the piping discipline might take control valves into account but it could also be seen as process control: important is to note that there are no double neither missing items.

Another vital aspect is to report exclusions to the scope. This is needed to have clear and undisputed boundaries of the scope. For example: in the case of BioSPRINT it is assumed that utilities are available at battery limits (the border of the process plant) and that infrastructural needs as roads, fences and buildings are present and large enough. Also, for example contaminated soil or underground obstacles at the building spot are excluded unless specifically mentioned.

7.4.3.2.3 Accuracy – reliability

Accuracy (accuracy is NOT a measure of estimate quality or estimate performance!); it is a measure of risk management; improve the risk identification, analysis and quantification, and treatment.

The estimating methodology used or required has a large impact on accuracy and quality of the estimates. There are two main categories to consider: stochastic and deterministic. Quite often a combination of the two is used, depending on the information available. Stochastic involves modelling, based on inferred or statistical relationships between costs and programming and/or technical parameters. Deterministic is more straightforward and counts or measures of units of items multiplied by known unit costs or factors. There are software applications available that allow for combining these methods and also offer their own embedded models like AspenTech software.

Since the estimating methodologies are another determining factor in producing reliable estimates, the experience and background of the estimator is also crucial. As the engineering phase of a project becomes more advanced, such as during the basic or detailed engineering phase, the methodology tends to become more deterministic. Mostly these estimates are executed by engineering companies that in the end also might lead the execution phase of a project. This requires the least experience or level of an estimator. The opposite case (that we in principle are dealing with in BioSPRINT) are mostly research and even early phase research cases where none to a maximum of 2 % of engineering has been performed. Methodologies here are mainly stochastic and expert system (in this case AspenTech) combinations that rely heavily on tuning/ tailoring by an experienced estimator. Also judging the system's outcome has to be reviewed against metrics as well as historic data. Since often in this stage of project development the process is still uncertain and only chemistry, determining and sizing equipment is a critical skill.

Sometimes it might even be that whole process sections will be adjusted from historic information that is available and it's up to the estimator's experience to judge validity of this.

Next to the obvious scope information as mentioned, equally important is to understand what the state of technology is and the quality of reference cost estimating data. Even when data is complete and percentage input info is high, this might be deceptive when for example technology is still uncertain, or "first of a kind" plant is built and maybe (as in BioSPRINT's case) R&D is still under way. Typically, if R&D is still not rounded, low accuracy is expected.

Quality of estimating reference data: for the BioSPRINT project there are a few items that are at the border of technical feasibility with respect to size. At the same time these are not off the shelf equipment items and very cost intensive. These should be checked with an equipment manufacturer in order to get more insight technically and price wise. This might the accuracy of the overall project significantly and should be done in when going from feasibility (class 5 AACE) to concept (class 4 AACE) according to [17], [18].

Other relevant factors related to accuracy will be reflected (but not discussed in detail here) are:

1. Time that is available to produce the estimate:
    a. Plan estimating like other disciplines. Often, only the end date is observed and estimating is squeezed
    b. Consider the type of estimate / experience / methodology / risks / unknowns (see also AACE RP 18R-97 [18]
2. Resources that are available:
    a. Obviously estimating resources like data and specialized estimator as mentioned earlier (Engineering resources, Laboratory resources, CFD and simulation resources)

All of the factors mentioned above pertain to the phase and the necessary level of accuracy or detail.

After completing the scope and exclusion paragraph, the estimate should be finalized by conducting a scope review to determine the level of scope definition. This in turn will be the base for a contingency estimate and will offer insight in challenges and improvement areas.

There are several types of contingency to be considered:

1. Technical contingency: to compensate for lack of scope definition. As scope develops further so does scope definition and contingency decreases. Scope changes, force majeure, warfare etc. are excluded from this.
2. Technological contingency: mostly related to new and unproven processes but could also be related to the size of a process.
3. Design and quantity allowances: covered in the base estimate, it is a function of the amount of design information that is available.

There are various methodologies to determine contingencies. When project development is already advanced it is best to make an in-depth analysis of risks, also considering project execution schedule, contracting strategy etc. next to obvious parameters such as scope, location, etc. A Monte Carlo based risk analysis would be good to assist with this but be aware that the whole project team should be involved and it's relatively time consuming. For projects as BioSPRINT where engineering is still at a very early stage proven tools like a FEL-index (Front-End Loading) can be used. This is basically a checklist to evaluate the scope completeness in a fast and proven way. The FEL-index will result in a number that corresponds with a percentage. This percentage is based on evaluation of several hundred projects that are evaluated before and after execution and of which the outcomes have been captured in a "index versus contingency percentage" graph.

7.4.4 Social assessment

The increased demand of integrating social aspects in life cycle assessments or sustainability assessments has led to the development of an international standard on social life cycle assessments (S-LCA) of products (ISO/DIS 14075). The S-LCA standard builds upon earlier work by UNEP [21] and [22], among others.

S-LCA is a method for evaluating the positive and negative social impacts of products (goods or services) along their respective life cycles. Since S-LCA has its origins in LCA, the two methods are closely aligned: S-LCA follows the classical four phases of LCA and additionally deals with (ideally the same) functional units and system boundaries. However, there are important methodological differences between S-LCA and LCA. First and foremost, this concerns the definition and selection of relevant stakeholders (categories) to which the subsequent assessment is tailored. Consequently, the overall results of the S-LCA are heavily dependent on this choice.

In contrast to other sustainability-related assessment methods (especially LCA), S-LCA is still clearly under development, but has evolved considerably over the past ten years. Owing to the method's infancy, it is hardly possible to identify specifically challenges when conducting an S-LCA study for products obtained via process-intensified manufacturing.

The main challenges include:

- Establishing a baseline ("reference", "business-as-usual", "current scenario", "counterfactual scenario", "conventional scenario", "status quo") against which the investigated process intensification is compared / benchmarked, especially if no established process exists.
- In S-LCA, the locations of life stages are of particular importance. Dedicated databases (e.g., Social Hotspots (SHDB) or Product Social Impact Life Cycle Assessment (PSILCA)) are available that provide generic information on social aspects in country-sector combinations. However, if both country and sector are the same (when comparing products obtained via process-intensified manufacturing with products obtained via non-intensified processes), no differences in terms of social risks and impacts might become apparent at the level of the foreground system. The background system (electricity generation, steel production etc.) might become more relevant, especially if the two compared systems differ considerably in terms of inputs.

7.4.5 Integrated sustainability assessment

In [23] and [24] the development of a Life Cycle Sustainability Assessment (LCSA) which is a method to quantify the sustainability impact of a product over its entire life cycle was developed. The method is derived from environmental life cycle assessment (LCA) and entails a sustainability assessment of products, originally coined in accordance with the three pillars of sustainability, while adopting a life cycle perspective. Since 2011, the Life Cycle Initiative promotes a pragmatic LCSA framework based on the three techniques [25]: LCSA = environmental life cycle assessment (LCA) + life cycle costing (LCC) + social life cycle assessment (S-LCA). In [26] the so-called integrated life cycle sustainability assessment (ILCSA) is proposed which – building upon existing frameworks – extends them with features for ex-ante assessments that increase the value for decision makers and introduces a structured discussion of results to derive concrete conclusions and recommendations. Due its strength in ex-ante assessments, it is well suited to be applied products obtained via process-intensified manufacturing.

The main challenges include:

- Alignment of and agreement on common definitions and settings, including system boundaries etc. (goal and scope definition).
- The life cycle inventory (LCI) analysis phase has to be split into two separate steps: The first step involves quantitative modelling of foreground processes, which is common for LCA, TEA and S-LCA and is based on complete mass and energy balances (see also section 7.3.2). The second is

the generation of impact-specific inventories from those models for each of the three assessment methods (e.g., yielding primary energy demand for LCA, energy costs for LCC and social impacts of energy provision for S-LCA).

- Choice of suitable indicators and delineation between the assessments contributing to the ILCSA
- Result integration

Please note that the currently developed technical standard on Eco-Technoeconomic Analysis (eTEA, ISO/WD TS 14076) does not qualify as a comprehensive sustainability assessment method, since it does not cover social aspects but only combines a techno-economic analysis (TEA) and a life cycle assessment (LCA) in a common framework.

8 Summary

The CEN Workshop Agreement (CWA) “EvaPIBioref” provides guidelines for evaluating the viability of process intensification (PI) measures in biorefining for manufacturers, owners, and engineers. It aims to assess whether PI offers a sustainable and cost-effective alternative to conventional, energy-intensive refining processes.

Despite its potential, the biorefinery sector faces significant processing and economic challenges, particularly with complex biomass feed streams. These streams may contain various impurities and inhibitors, complicating conversion and purification processes, leading to low yields and product quality. Process intensification strategies can offer solutions to these challenges. Benefits include lower energy consumption, reduced waste and safety risks, leading to higher process efficiency and environmental sustainability across the biorefinery process.

The three options of PI are innovative technologies, processing methods, and materials like catalysts or solvents. PI combines elements from this ‘PI toolbox’ to significantly reduce processing equipment volume, often by one to two orders of magnitude. enabling compact devices with larger surface areas to facilitate better mixing and transfer rates.

Key items provided in the workshop agreement for the evaluation of PI of biorefining processes are:

- Identification and description of the framework to be considered, which consist of:
    - A discussion of the drivers for process intensification
    - Comprehensive listings on intensified process equipment, intensification methods, and materials along with descriptions of principles, the target limiting steps, possible applications and limitations.
    - Training and education needs
- A methodological framework for conducting a PI assessment of biorefinery processes which consists of
    - A step-by-step iterative procedure centred around knowledge-based engineering to understand the whole process from raw material purification through to final product, identify rate limitation steps and select targeted PI strategies to match process requirements. The drivers for embarking on this journey of change or improvement should be clearly identified from the outset, which would likely be guided by TEA or LCA considerations.
    - Description of process modelling and simulation principles for early identification of technology limitations, risks and improvement opportunities. These steps include (i) the definition of system boundaries and modelling scope, (ii) mass and energy balance calculations, (iii) data acquisition and the choice of thermodynamic property models with regard to PI and the handling of uncertainties, followed by (iv) simulation of upscaling.

- Description of the sustainability assessment based on life-cycle approaches, which play an increasingly significant role for setting performance criteria. Three methods for assessing the environmental, economic and social performance of products are introduced: (i) The principles of life cycle assessment, which addresses the environmental aspects and potential environmental impacts throughout a product's life cycle; (ii) The principles of the techno-economic analysis are here described using items from the European research project "Biorefining of sugars via Process Intensification – BioSPRINT"; (iii) The principles of social life cycle assessments, which is a method for evaluating the positive and negative social impacts of products along their respective life cycles. Finally, the approach to an (iv) integrated sustainability assessment is outlined. Its aim is to increase the value of the assessment for decision makers by deriving concrete conclusions and recommendations.

Bibliography

[1] Panoutsou, C., Pantaleo, M., Dees, M., Berien, E., Iriarte, L., Fritsche, U., Glavonjic, B., Stojadinovic, D., Zhelyezna, T., Carrez, D., 2016. D8.1 Overview report on the current status of biomass for bioenergy, biofuels & biomaterials in Europe.

[2] Ramshaw, C., 1999. Process Intensification and Green Chemistry. Green Chem. 1, G15–G17. https://doi.org/10.1039/gc990g15

[3] Wang, H., Mustaffar, A., Phan, A.N., Zivkovic, V., Reay, D., Law, R., Boodhoo, K., 2017. A review of process intensification applied to solids handling. Chemical Engineering and Processing: Process Intensification 118, 78–107. https://doi.org/10.1016/j.cep.2017.04.007

[4] Boodhoo, K.V.K., Flickinger, M.C., Woodley, J.M., Emanuelsson, E.A.C., 2022. Bioprocess intensification: A route to efficient and sustainable biocatalytic transformations for the future. Chemical Engineering and Processing - Process Intensification 172, 108793. https://doi.org/10.1016/j.cep.2022.108793

[5] Fernandez Rivas, D., Boffito, D.C., Faria-Albanese, J., Glassey, J., Afraz, N., Akse, H., Boodhoo, Kamelia.V.K., Bos, R., Cantin, J., (Emily) Chiang, Y.W., Commenge, J.-M., Dubois, J.-L., Galli, F., De Mussy, J.P.G., Harmsen, J., Kalra, S., Keil, F.J., Morales-Menendez, R., Navarro-Brull, F.J., Noël, T., Ogden, K., Patience, G.S., Reay, D., Santos, R.M., Smith-Schoettker, A., Stankiewicz, A.I., Van Den Berg, H., Van Gerven, T., Van Gestel, J., Van Der Stelt, M., Van De Ven, M., Weber, R.S., 2020a. Process intensification education contributes to sustainable development goals. Part 1. Education for Chemical Engineers 32, 1–14. https://doi.org/10.1016/j.ece.2020.04.003

[6] Fernandez Rivas, D., Boffito, D.C., Faria-Albanese, J., Glassey, J., Cantin, J., Afraz, N., Akse, H., Boodhoo, K.V.K., Bos, R., Chiang, Y.W., Commenge, J.-M., Dubois, J.-L., Galli, F., Harmsen, J., Kalra, S., Keil, F., Morales-Menendez, R., Navarro-Brull, F.J., Noël, T., Ogden, K., Patience, G.S., Reay, D., Santos, R.M., Smith-Schoettker, A., Stankiewicz, A.I., Van Den Berg, H., Van Gerven, T., Van Gestel, J., Weber, R.S., 2020b. Process intensification education contributes to sustainable development goals. Part 2. Education for Chemical Engineers 32, 15–24. https://doi.org/10.1016/j.ece.2020.05.001

[7] Reay, D.A., Ramshaw, C., Harvey, A., 2013. Process intensification: engineering for efficiency, sustainability and flexibility, Second edition. ed. Butterworth-Heinemann, Oxford.

[8] Teoh, S.K., Feng, R., Tan, B., Ramchandani, S.R., Boodhoo, K.V.K., Sharratt, P., 2015. A methodology to evaluate pharmaceutical and fine chemicals processes for intensification and sustainability benefits, in: 5th European Process Intensification Conference (EPIC). Nice, France.

[9] Teoh, S.K., Rathi, C., Sharratt, P., 2016. Practical Assessment Methodology for Converting Fine Chemicals Processes from Batch to Continuous. Org. Process Res. Dev. 20, 414–431. https://doi.org/10.1021/acs.oprd.5b00001

[10] Sharifian, S., Sotudeh-Gharebagh, R., Zarghami, R., Tanguy, P., Mostoufi, N., 2021. Uncertainty in chemical process systems engineering: a critical review. Reviews in Chemical Engineering 37, 687–714. https://doi.org/10.1515/revce-2018-0067

[11] Balgobin, T., Evrard, D., 2020. A framework for modelling emerging processes' upscaling from an environmental perspective. Procedia CIRP, 27th CIRP Life Cycle Engineering Conference

(LCE2020) Advancing Life Cycle Engineering: from technological eco-efficiency to technology that supports a world that meets the development goals and the absolute sustainability 90, 154–158. https://doi.org/10.1016/j.procir.2020.01.055

[12] UNFCCC, 2015. The Paris Agreement. United Nations Framework Convention Climate Change.

[13] Persson, L., Carney Almroth, B.M., Collins, C.D., Cornell, S., De Wit, C.A., Diamond, M.L., Fantke, P., Hassellöv, M., MacLeod, M., Ryberg, M.W., Søgaard Jørgensen, P., Villarrubia-Gómez, P., Wang, Z., Hauschild, M.Z., 2022. Outside the Safe Operating Space of the Planetary Boundary for Novel Entities. Environ. Sci. Technol. 56, 1510–1521. https://doi.org/10.1021/acs.est.1c04158

[14] Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F.S., Lambin, E.F., Lenton, T.M., Scheffer, M., Folke, C., Schellnhuber, H.J., Nykvist, B., De Wit, C.A., Hughes, T., Van Der Leeuw, S., Rodhe, H., Sörlin, S., Snyder, P.K., Costanza, R., Svedin, U., Falkenmark, M., Karlberg, L., Corell, R.W., Fabry, V.J., Hansen, J., Walker, B., Liverman, D., Richardson, K., Crutzen, P., Foley, J.A., 2009. A safe operating space for humanity. Nature 461, 472–475. https://doi.org/10.1038/461472a

[15] Steffen, W., Richardson, K., Rockström, J., Cornell, S.E., Fetzer, I., Bennett, E.M., Biggs, R., Carpenter, S.R., De Vries, W., De Wit, C.A., Folke, C., Gerten, D., Heinke, J., Mace, G.M., Persson, L.M., Ramanathan, V., Reyers, B., Sörlin, S., 2015. Planetary boundaries: Guiding human development on a changing planet. Science 347, 1259855. https://doi.org/10.1126/science.1259855

[16] Wang-Erlandsson, L., Tobian, A., Van Der Ent, R.J., Fetzer, I., Te Wierik, S., Porkka, M., Staal, A., Jaramillo, F., Dahlmann, H., Singh, C., Greve, P., Gerten, D., Keys, P.W., Gleeson, T., Cornell, S.E., Steffen, W., Bai, X., Rockström, J., 2022. A planetary boundary for green water. Nat Rev Earth Environ 3, 380–392. https://doi.org/10.1038/s43017-022-00287-8

[17] AACE, 1997a. AACE International Recomended Practice No. 17R-97: Cost estimate Classification System. Association for the Advancement of Cost Engineering.

[18] AACE, 1997b. AACE International Recomended Practice No. 18R-97: Cost estimate Classification System – as applied in Engineering, Procurement, and Construction for the Process Industries. Association for the Advancement of Cost Engineering.

[19] Richardson Engineering Services, 1996. Richardson’s international construction factors : location cost manual. Richardson Engineering Services, Mesa, Ariz.

[20] Compass International Inc., 2024. Construction Cost Estimating Data [WWW Document]. URL https://compassinternational.net/

[21] UNEP, 2020. Guidelines for Social Life Cycle Assessment of Products and Organisations 2020. United Nations Environment Programme. https://wedocs.unep.org/20.500.11822/34554

[22] Goedkoop, M.J., Beer, I.M. de, Harmens, R., Saling, P., Morris, D., Florea, A., Hettinger, L., Indrane, D., Visser, D., Morao, A., Musoke-Flores, E., Alvarado, C., Rawat, I., Schenker, U., Head, M., Collotta, M., Andro, T., Viot, J.-F., Whatelet, A., 2020. Product Social Impact Assessment Handbook. Amersfoort, November 1st, 2020.

[23] Kloepffer, W., 2008. Life cycle sustainability assessment of products: (with Comments by Helias A. Udo de Haes, p. 95). Int J Life Cycle Assess 13, 89–95. https://doi.org/10.1065/lca2008.02.376

[24] Finkbeiner, M., Schau, E.M., Lehmann, A., Traverso, M., 2010. Towards Life Cycle Sustainability Assessment. Sustainability 2, 3309–3322. https://doi.org/10.3390/su2103309

[25] UNEP, 2011. Towards a life cycle sustainability assessment: making informed choices on products. United Nations Environment Programme. https://wedocs.unep.org/20.500.11822/8001

[26] Keller, H., Rettenmaier, N., Reinhardt, G.A., 2015. Integrated life cycle sustainability assessment – A practical approach applied to biorefineries. Applied Energy 154, 1072–1081. https://doi.org/10.1016/j.apenergy.2015.01.095

[27] World Commission on Environment and Development (Ed.), 1987. Our common future, Oxford paperbacks. Oxford University Press, Oxford; New York.