Resource efficiency indicator-based decision support for the operation of batch and mixed batch-continuous processing plants

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Kurzfassung

Steigende Konzentrationen von Treibhausgasen in der Atmosphäre sind der Grund für den globalen Klimawandel. Da die chemische Industrie wesentlich zu den Treibhausgasemissionen beiträgt, schaffen politische Entscheidungsträger Anreize und Gesetze, um die Industrie zu einer nachhaltigeren Produktion zu bewegen. In dieser Arbeit wird ein Rahmen zur Definition und Nutzung von Echtzeit-Ressourceneffizienzindikatoren (REI) entwickelt, um die Ressourceneffizienz industrieller Produktionsprozesse kontinuierlich zu überwachen und zu optimieren. Die Ressourceneffizienz ist eine mehrdimensionale Größe, die in Relation zur Wirtschaftlichkeit bewertet werden kann. Der Fokus der Arbeit liegt dabei auf Batch-Prozessen und Prozessen, die diskontinuierliche und kontinuierliche Teilprozesse kombinieren. Diese stellen eine Herausforderung für die korrekte Erfassung relevanter Prozessgrößen und die anschließende Analyse dar. Das vorgeschlagene Propagationskonzept ermöglicht es, den Gesamtwirkungsgrad der Anlage auf Basis der Leistung ihrer Komponenten zu berechnen. Die daraus resultierenden REIs spiegeln die technische Leistung der Anlage wieder und werden zur Optimierung der gesamten Ressourceneffizienz eines Anwendungsbeispiels verwendet. Die Optimierung der Ressourceneffizienz stellt ein mehrdimensionales Optimierungsproblem dar, bei dem die Pareto-optimalen Betriebspunkte die möglichen Kompromisse zwischen konkurrierenden Interessen angeben. Die Auswahl eines gewünschten Betriebspunktes aus der Paretomenge ist nicht trivial und kann sich ändernden Präferenzen folgen. Daher befasst sich der zweite Teil der Arbeit mit der Synthese eines effizienten und effektiven Entscheidungsunterstützungssystems (Decision Support System, DSS) zur Auswahl eines Betriebspunktes mit dem gewünschten Leistungsprofil. Die Methodik wird auf ein Beispiel angewendet und durch eine experimentelle Usability-Studie validiert. Damit leistet diese Arbeit einen Beitrag zur Optimierung der Ressourceneffizienz in der Prozessindustrie durch die Identifikation von ressourcenoptimalen Betriebszuständen. Die ganzheitliche Betrachtung der Ressourceneffizienz in Batchprozessen stellt eine wichtige Erweiterung der industriellen Praxis dar, die sich derzeit in der Regel auf eine Energieeffizienzanalyse nach ISO50001 beschränkt.

Abstract

Increasing concentrations of greenhouse gases (GHG) in the atmosphere are the reason for global climate change. Since the chemical industry is a significant contributor to the GHG emissions, policy makers are creating incentives and legislation to steer the industry towards a more sustainable production. This thesis proposes a framework to define and utilize real-time resource efficiency indicators (REI) to constantly monitor and optimize the resource efficiency of industrial production processes. Resource efficiency is a multi-dimensional entity that can be evaluated in relation to the economic performance. The focus of the thesis is on batch- and hybrid – coupled batch and continuously operated – processes that introduce further challenges for the correct recording of relevant process variables and the subsequent analysis. The proposed propagation concept makes it possible to calculate the overall efficiency of the plant based on the performance of its components. The resulting REIs reflect the technical performance of the plant and are used to optimize the overall resource efficiency of an application case. Optimizing the resource efficiency of a process poses a multi-dimensional optimization problem, where the Pareto optimal operating points reflect the potential trade-offs between competing interests. The selection of a desired operational point among the optimal set is not trivial and may be subject to changing preferences. Thus, the second part of the thesis addresses the synthesis of an efficient and effective decision support system (DSS) to select an operating point with the desired performance profile. The methodology is applied and validated by an experimental usability-study. In summary, the thesis contributes to the optimization of resource efficiency in the process industry by identifying resource-optimal operating conditions. The holistic consideration of resource efficiency in batch processes represents an important extension of industrial practice, which is up to now usually limited to an energy efficiency analysis according to ISO50001.

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Chapter 1

Introduction

One of the current challenges for the global community is to fight climate change, which is caused by a growing concentration of greenhouse gases (GHG) in the atmosphere (Abbass et al., 2022). The greenhouse effect is intensified by industrial emissions and the excessive use of fossil fuels in combustion processes. For the processing industry two contribution mechanisms are relevant. Primary emissions are the direct result of chemical reactions, where all or some of the stoichiometric side products are GHG. Secondary emissions are not emitted within the process boundaries, but are related to transport activities, the raw materials or energy use. Thus, the processing industry can contribute to the reduction of GHG emissions by using alternative reaction routes, substituting raw materials with renewable alternatives, and improved resource efficiency.

The entire industrial production in Germany accounts for 28.5% of the total primary energy use, of which 29.3% are contributed by the chemical industry (Energy, 2021; Destatis, 2021). Therefore, policy makers have identified the chemical industry as one of the major potential contributors to a reduction of the causes of global warming. The impact assessment "Stepping up Europe's 2030 climate ambition" is the newest in a series[1] of communications that raised the emission reduction targets by the European Commission. It imposes targets on the reduction of GHG emissions of 55%) compared to the reference year 1990.

The climate strategy packages of the European Commission are a binding commitment of the member states to achieve the goals. However, the decisions and directives do not specify how to achieve the targets on a national level. The German government decided to grant partial tax exemption to companies that implement energy management systems according to the ISO50001 standard, to motivate companies to continuously improve

[1] The "2020 climate and energy package" was the first package implementing targets and legislation within the European Union (Decision No 406/2009/EC; Directive 2009/28/EC; Directive 2009/29/EC; Directive 2009/31/EC). In September 2020 an impact assessment was published by the European Commission that further increased the 2030 targets on the way to the 2050 long term goal of net-zero greenhouse gas emissions (COM, 2018; SWD, 2020).

their energy efficiency (Gleich, 2014; ISO50001:2018).

There are numerous efforts of standardization bodies to define uniform indicators to measure the efficiency of industrial processes with different objectives in mind. Energy Management Systems (EnMS) according to the ISO50000-series and Environmental Management Systems following the methodology of the ISO14000-series are globally established frameworks to measure resource efficiency related factors. Section 2.1 describes the frameworks relevant for this thesis. The majority of the standards aim to capture and report the performance of an organization, typically in intervals of one year. This enables companies to benchmark their process performance against a reference in order to monitor the continuous improvement and to evaluate the effectiveness of implemented measures. The ISO50002:2014 standard (Energy Audits) contains some guidance on how to identify improvement potentials within an organization. Since the ISO50000 framework is intended to be generally applicable to a broad variety of organizations, the guidance is of limited use for operational issues in the process industry. Among other factors, the way a production plant is operated can make an important contribution to resource efficiency. The plant personnel has some degrees of freedom in the operating window, which they usually use to ensure a smooth operation at high throughput. These degrees of freedom can be used to improve resource efficiency by determining and using an optimal set of input parameters. However, this is not trivial, as external influences such as ambient temperature, raw material qualities and sales capacities influence the optimal operating point. To realize this potential, three factors are important: (1) Indicators must be available to measure the efficiency of the plant in near real-time, (2) the effect of external influences must be adjusted, and (3) the results of an analysis or optimization must be made available to the user in the form of a decision support system.

These requirements were the starting point and motivation for this thesis and the MORE[2] project, which was funded within the 7th framework programme of the European Union (call FP7-NMP-2013-SMALL-7). Within the same call two other projects were funded that shared the goal of improving the industrial resource efficiency, but took different approaches to achieve this goal. The REFFIBRE project[3] focused on the pulp and paper industry and defined indicators for the economic, environmental and technological process performance on the company or site level (Leon et al., 2016). The derived indicators were evaluated using state-of-the-art Life Cycle Assessment (LCA) tools to compare the process performance with reference values. The project results show that indicator-based analyses of the product life cycle and of the industry involved can be used to identify synergy effects through process integration. However, it is not possible to improve the

[2]Title: "Real-time Monitoring and Optimization of Resource Efficiency in Integrated Processing Plants (MORE)"

[3]Title: "Tools for Resource-Efficient use of recycled FIBRE materials (REFFIBRE)"

operation of individual plants with this method. The project TOP-REF[4] derived key resource indicators (KRI) for the material, energy and water consumption on the process level (CIRCE, 2014). The indicators can be aggregated to a single global measure based on the exergy values of the process streams and to optimize processes with respect to the individual KRI or the combined measure based on exergy (Radatz et al., 2019a,b). In principle, it is possible to use this exergy-based method to optimize plant operations. However, it has some disadvantages in industrial applications. The method makes it necessary to evaluate all relevant process streams across the system boundary according to their exergy. This requires knowledge about their composition, temperature, pressure and the exergy values of the raw materials. This information is expensive to obtain and difficult to interpret. The strengths of this method lie rather in the identification of process streams that still contain usable energy and can be used for process integration.

The methods developed in this thesis were developed in the scope of the MORE and the subsequent CoPro[5] project and extend the methodology by deriving real-time resource efficiency indicators for plants operated in batch and continuous mode in the process industry. Furthermore, the indicators are used to formulate and solve optimization problems targeting the resource efficiency of industrial application cases by supplying valuable and effective decision support to plant personnel.

1.1 Challenges

The definition and selection of meaningful real-time resource efficiency indicators (REI) that cover all relevant factors of resource efficiency is not a trivial task. The process industry uses a large number of different production processes and unit operations to convert raw materials into valuable products by means of chemical or biological processes. Typically, the reaction products must be further separated to ensure the required product purity. A resource efficiency optimization framework must be generally applicable to a wide range of industrial sectors. Furthermore, different operating modes are common, which call for tailored strategies to record, process and evaluate the information necessary to calculate the REIs. The most prominent distinction is made between continuously operated processes and those which are carried out in batch operation, while hybrid or mixed forms can occur. After the indicators have been defined, it is necessary to test their applicability for resource efficiency optimization. The procedure should be standardized as much as possible to ensure that weaknesses are detected before the indicators are implemented. Furthermore, production processes typically consist of multiple production

[4] Title: “Innovative tools, methods and indicators for optimizing the resource efficiency in process industry (TOP-REF)”

[5] Title: “Improved energy and resource efficiency by better coordination of production in the process industries (CoPro)”

stages and are highly integrated with other processes to conserve energy and materials. Thus, a comprehensive methodology is needed to aggregate the efficiency of subsystems to the overall performance, in order to find the global optimum.

The definition of resource efficiency considers it as a multidimensional quantity of energy efficiency, material efficiency and environmental performance (Kalliski and Engell, 2017). Thus, trade-offs between the different efficiency metrics may arise. For example, it is usually possible to improve the environmental efficiency at the expense of energy efficiency by means of energy-intensive after-treatment of waste water or exhaust gases. Thus, optimizing the resource efficiency translates to solving a multi-dimensional optimization problem (MDOP). The optimal solution of an MDOP is the Pareto frontier (Pareto, 2014), which is the set of operating points that cannot be improved for one objective without worsening another. It can either be obtained from an extensive amount of process data or from model-based approaches. The data-based approach evaluates the operating regime as recorded in the historical process data and approximates the Pareto front in the efficiency indicator space by fitting a function to the boundary of historical operating points towards improved objectives. Beisheim et al. (2019) implemented a robust k-means approach to obtain an approximation of the Pareto frontier. However, it is challenging to identify the process inputs that would achieve the efficiencies corresponding to a point on the Pareto set. Furthermore, the data-based approach can only identify operational states that were achieved before. Model-based approaches are initially more complex to implement, but provide the input parameters that lead to an optimal solution and can identify the true Pareto set. But even here it is challenging to obtain a uniform distribution and good coverage of the Pareto front, especially for non-convex problems. If the Pareto front is available, operators and plant managers can select an operating point among the Pareto set that suits their preferences. Pareto-optimal operating points with respect to resource efficiency are a valuable reference to monitor the performance of a chemical or biochemical production process. Integrating this information into computer-based decision support systems (DSS) can help plant mangers and shift personnel to actively improve the resource efficiency.

The next challenge on the way to an efficient decision support solution is the design of the human machine interface (HMI) that acts as an interface between the system and the decision maker. A good understanding of the process and the resulting Pareto frontier can only be achieved with little effort if the depicted information is clear, precise and easy to understand. A tailored HMI design is needed that suits the informational needs of the decision making process, while minimizing the amount of information on the dashboard (Tufte, 2006; Rasmussen and Vicente, 1989). Revisiting the differences between batch-wise and continuously operated plants highlights the consequences for the selection of visualization elements: while continuous plants are more or less in steady-state and their efficiency can be comprehended as system wide state, in batch processes distinct units of material travel through the plant that posses different efficiencies. Furthermore, batch processes inherently have time as an additional degree of freedom. Their efficiency is often dependent on the total reaction time, the material inputs, and the temperature profile resulting from heating or cooling. This increases the complexity of the Pareto navigation and must be considered during the design of the HMI. Finally, technological hurdles need to be overcome to implement a responsive and performant DSS solution that avoids frustrating the user. A pleasant user experience increases the likelihood that the user will regularly consult the DSS, maximizing the positive impact on resource efficiency.

1.2 Objective and approach

The overarching goal of this thesis is to support the industry to optimize the resource efficiency of production processes. This target can be broken down into the following objectives:

1. Develop a framework to define, evaluate and obtain real-time REI for batch and mixed batch-continuous processes. They must be sensitive to the technical resource efficiency performance for a broad variety of production processes.
2. Derive a methodology to aggregate local performance measures to a plant wide efficiency indicator.
3. Develop a strategy to solve the resulting optimization problems for the one- and multi-dimensional case, in order to find the global optimum or the set of Pareto-optimal solutions.
4. Identify suitable visualization elements to display the resource efficiency performance for batch-wise and continuously operated production processes.
5. Assemble decision support solutions to effectively monitor the process performance and enable the user to select the best operating point among the set of optimal solutions.

Based on the state-of-the-art in **Chapter 2** the framework for the development of real-time REI for batch processes is developed in **Chapter 3**, with particular emphasis on the challenges that are associated with batch processes. The resulting method is applied to an application case to find the energy optimal operating point of a sugar plant with partially batch-wise and continuous operation.

Chapter 4 considers the multi-dimensional case, in which the individual contributions to resource efficiency are separately considered and optimized for the Williams-Otto semi-batch reactor example. In the multi-dimensional case the optimum is a set of Pareto-optimal operating points that poses great challenges for an effective and efficient visualization of the Pareto-frontier. The design process of decision support solutions for the multi-dimensional case in the context of batch processes is described in **Chapter 5**. The development of this scalable DSS is pioneering work in the field of optimal indicator-based decision support. To prove the efficiency and effectiveness of the system, an experimental usability study is performed on an interactive implementation of the DSS in **Chapter 6**. Finally, **Chapter 7** summarizes the findings and provides an outlook on remaining challenges.

Chapter 2

State of the art

The description of an organization's resource efficiency by KPIs is well established and generally aims at a retrospective reporting system through which companies communicate the impact of their economic processes on the environment. This chapter provides an overview of applicable standards, related frameworks and their shortcomings in describing resource efficiency for production plants in the process industry. Subsequently, the basics for the definition of real-time resource efficiency indicators and the selection of a suitable set of indicators that fully describe resource efficiency are described. These principles were developed by the author in cooperation with the project partners of the research project MORE[1].

2.1 Standardization and reporting of indicators

The overview given in this section is based on the summary assembled by Lieback et al. (2018) and Kujanpää et al. (2018). Relevant to the area of resource efficiency are the ISO14000- and ISO50000-standards. While the ISO14001:2015 covers Environmental Management Systems (MS), the ISO50001:2018 focuses at Energy MS.

2.1.1 ISO14000 series

Environmental Management Systems compliant with ISO14001:2015–ISO14006:2011 can be used to manage the resource efficiency of an organization. The scope of the management efforts can be divided into the resource usage within the organization and impacts that act outside of the organizations boundary. The Material Flow Cost Accounting (MFCA) is a framework to track and optimize material flows within an organization based on physical measures, also taking into account the associated costs (ISO14051:2011). If successfully applied, MFCA reduces emissions and waste management costs. The other

[1] "Real-time Monitoring and Optimization of Resource Efficiency in Integrated Processing Plants (MORE)"

standards within the series focus on external factors, e.g. the Life Cycle Analysis (LCA) that evaluates all stages of a products life from the raw materials to the final disposal of the product (ISO14040:2006; ISO14044:2006). The eco-efficiency assessment described in ISO14045:2012 evaluates the environmental performance of a product in relation to it's value, in order to support the decision making process during the product and supply chain design. Finally, the footprint standards ISO14067:2018 and ISO14046:2014 help to assess the carbon and water footprint respectively.

2.1.2 ISO50000 series

The ISO50000-series defines the requirements and guidelines to implement energy management systems (EnMS). The central standard ISO50001:2018 is extended by guidelines on the implementation of EnMS (ISO50004:2014) and the definition of Energy Performance Indicators (EnPI) that are used to measure the performance of organizations (ISO50006:2014). The ISO50002:2014 contains an approach to internal energy audits that collect energy data and information for the calculation of the energy baseline and EnPI. Based on the collected information, the plan-do-check-act cycle approach is used to continuously improve the energy efficiency of the organization. The ISO50003:2014 determines on what basis the certification bodies can issue a certificate (see fig. 2.1). The renewed version of the ISO50001 extends the requirements for certification. The EnPIs must be corrected by external influences such as ambient temperature and production load. Furthermore, a continuous improvement of the energy efficiency is necessary to be recertified each year. This is done with respect to a reference state, called Energy Baseline.

According to the ISO survey, most ISO50001 certificates were awarded to German organizations in 2019, with a share of 31.7% (ISO Survey, 2019). The second place is held by China with a share of 16.1% of the total 18,227 certificates awarded worldwide. The success in Germany is due to the reimbursement on electricity and energy taxes, according to the tax cap efficiency regulation (SpaEfV[2]). In order to be eligible for the tax reimbursements an EnMS must be in place and certified with respect to the ISO50001 standard. In addition to tax refunds, a study conducted by Offermann et al. (2013) found that EnMS based on ISO50001 are effective to achieve energy savings, thus, having an impact on CO_2 emissions and energy costs.

2.1.3 Reporting mechanisms

Kujanpää et al. (2018) distinguishes between obligatory and voluntary reporting of resource efficiency information. Both approaches aim at introducing a certain level of trans-

[2]Spitzenausgleich-Effizienzsystemverordnung, published on 31.07.2013, on the basis of §66 EnergieStG and §12 StromStG

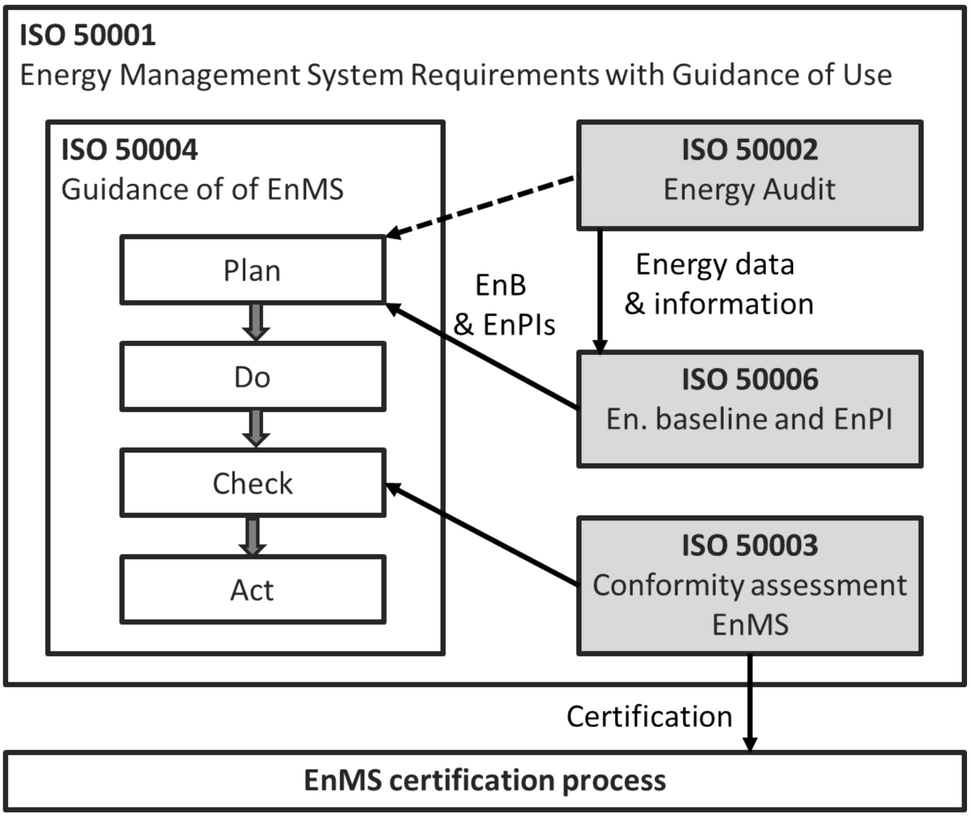

Figure 2.1: Organizational relations of standards in the ISO50000-series. Adapted from Lieback et al. (2018).

parency for industrial processes by making information about emissions and environmental impact publicly available allows for the assessment and benchmarking of industrial processes. The resulting transparency enables the governing bodies to impose legislation that creates incentives or requirements regarding the resource efficiency of production facilities. In recent years, the awareness for the impact of the industry on climate change has grown. Thus, implementing and advertising efforts to improve the energy and resource efficiency of production processes has become more and more important to create a favorable public image of corporations.

Obligatory reporting

The obligatory reporting comprises the EU Directive on Industrial Emissions (IED) and the EU Directive on Non-financial Reporting.

The Directive 2014/95/EU on Non-financial Reporting requires organizations in excess of 500 employees to publish information on the social and environmental impacts, together with an assessment of the associated sustainability risks. The directive is not specific on how to prepare the data and what to include, but rather lists frameworks that have acceptable procedures. These include: the Eco-Management and Audit Scheme (EMAS, 2019), the OECD Guidelines for Multinational Enterprises (OECD, 2011), the UN Global Compact (UNGC, 2015), the ISO26000:2010, and the Global Reporting Initiative (GRI, 2020).

The Directive 2010/75/EU on Industrial Emissions aims to "achieve a high level of protection of human health and environment by reducing harmful emissions across the European Union", by an integrated approach that must take into account the environmental performance of the plant, emissions, waste, raw material consumption, and energy efficiency. The related European pollutant release and transfer register (E-PRTR, 2020) manages a database that is used to publish the annual emission data of industrial facilities across Europe.

Voluntary reporting

The voluntary reporting includes the Eco-Management and Audit Scheme (EMAS), the OECD Guidelines for Multinational Enterprises, the UN Global Compact, and the Global Reporting Initiative (GRI).

The EMAS should encourage companies to continuously improve their environmental performance through measuring, evaluating, reporting, and improving their processes (EMAS, 2019). The indicators listed to assess the performance are

- energy efficiency,
- material efficiency,
- water consumption,
- waste generation,
- biodiversity,
- and air emissions (e.g. GHG emissions).

The European Commission specifies that the indicators must be sector-specific to allow for a benchmarking among plants of similar nature. Most activities target company internal processes, e.g. audits, but an environmental statement must be made publicly available.

The OECD Guidelines for Multinational Enterprises (OECD, 2011) provide non-binding principles and standards to positively contribute to the economic, environmental and social progress across country boarders. The emphasis of the guidelines is on the compliance with socio-economic rules to ensure a fair competition and development. In addition the environmental performance is mentioned and should be evaluated throughout the entire life cycle. Similar to the EU Directive on Non-financial Reporting (Directive 2014/95/EU) the reporting mechanisms are not specified within the Guidelines, but referrals to the Global Reporting Initiative or ISO-certified management systems are mentioned (see ISO9001:2015; ISO14001:2015; ISO50001:2018).

The United Nation's Global Compact Initiative (UNGC, 2015) has a similar scope to the OECF Guidelines mentioned before. Following the analysis of Kujanpää et al. (2018), three principles within the initiative are relevant for resource efficiency considerations:

Principle 7: Businesses should support a precautionary approach to environmental challenges that involves a discourse between all stakeholders.

Principle 8: Businesses should undertake initiatives to promote greater environmental responsibility. On the one hand, the efforts should be oriented towards internal processes to encourage employees to innovate and improve the processes. On the other hand, it should also include a transparent external communication to benchmark against the peers.

Principle 9: The business should encourage the development and diffusion of environmentally friendly technologies. This principle does focus on the required technological solutions to supplement the organizational efforts mentioned in principle 8.

In addition to the adhering to the defined principles, the UN Global Compact Initiative requires companies to deliver Communications on Progress (COP) to the Global Compact database. This report can be stand-alone or be issued in the scope of other reporting schemes.

The fourth reporting scheme that is relevant for the resource efficiency of production processes is the GRI, 2020. It includes a broad variety of Guidelines from the categories

- economic,
- environmental,
- and social, with the subdivisions labor practices and decent work, human rights, society and product responsibility.

The methodology encourages to focus on the most pressing topics within an organization. An extensive overview over the guidelines relevant for resource efficiency can be found in Kujanpää et al. (2018).

2.1.4 Shortcomings of existing indicators and systems

Most of the indicators discussed so far focus on reporting and cannot be directly used to identify improvement potentials or real-time optimization of production processes. This holds especially true for the methods mentioned in section 2.1.3. The management systems covered in the ISO14000- and ISO50000-series are more process centered, but they are still lacking real-time applicability and suitability for process optimization. In the given context, real-time applicability refers to the time frame for operational decisions. Typically, decisions regarding resource efficiency are performed on a batch-to-batch or day-to-day timescale. Conventional resource efficiency indicators are calculated in retrospect for the previous months to years and are not suitable to steer the resource efficiency of a production plant in real time. Furthermore, practical considerations on how to prepare and visualize the indicators best is often overlooked. To increase the impact on day-to-day operations an integrated methodology is needed that can assess energy, material, and eco-efficiency at the same time and deliver tailored decision support solutions.

2.2 Resource efficiency indicator framework

The introduction of this section and large parts of subsections 2.2.1–2.2.2 have been published in Kalliski and Engell (2017)[3] *and Beisheim et al. (2018)*[4]*. Large parts of section 2.2.3 were published in Beisheim et al. (2018)*[4]*.*

Considerable efforts have been made in the past to improve the resource efficiency of chemical production plants in order to secure the competitiveness of the existing production facilities and to improve the sustainability of chemical production (Cefic 2013). Key performance indicators (KPIs) are widely used to report the environmental impacts and production performance on the company level. Energy performance indicators (EnPIs) as required by the ISO standard 50001 were designed to assess the effectiveness of energy management (ISO50001:2018). Furthermore, standards from the ISO14000 series define environmental indicators for environmental management systems (ISO14001:2015). They provide guidelines for eco-design (ISO14006:2011), life cycle assessment (ISO14040:2006; ISO14044:2006), and to measure the carbon and water footprints (ISO14067:2018; ISO14046:2014). Indicators defined in these standards are typically calculated in retrospect and over long time horizons. They are suitable to measure the effect of changes in the plant technology, in the product and raw-material portfolio, and in the operating policies. Due to the temporal aggregation of months or years, they are, however, not suitable for decision support and optimization of the processes during daily operations.

In this thesis, resource efficiency is seen as a multi-dimensional entity that encompasses the performance with respect to energy, material, and environmental aspects. Many approaches to improve different aspects of resource efficiency and to reduce the environmental impact have been reported in the literature (Baños et al., 2011). Often, the improvement of resource efficiency is targeted towards a single key indicator that was identified as

[3]Reproduced with permission, ©2016 Canadian Society for Chemical Engineering

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the main cost factor, while maintaining a desired production rate, e.g. the minimization of steam consumption or the maximization of material efficiency (Oldewurtel et al., 2012; Ji et al., 2013). However, improving only one of the factors that contribute to the resource efficiency of a production process does not ensure an economically optimal or overall resource efficient production. Economic optimization approaches, in contrast, maximize the total profit considering the costs associated to the streams of energy and materials as well as the revenues created by the product output in one objective function. Economic approaches are well established for a multitude of industrial application cases and optimization strategies (Engell, 2007; Trierweiler, 2013), e.g. economic-based model predictive control (Amrit et al., 2011; Idris and Engell, 2012), but with a growing pressure from the legislators and society it becomes important to include considerations regarding resource efficiency that cannot be directly translated to financial values. Thus, it is proposed to define resource efficiency indicators (REI) that reflect

- the energy efficiency,
- the material efficiency,
- and the environmental performance

of industrial processes and consider them in conjunction with

- the economic benefit.

In this chapter, the measurement and improvement of resource efficiency during daily operations of plants in the process industries is addressed, in particular of plants with a significant element of batch operations. Operational policies, i.e. how the operational degrees of freedom of a plant are set when the plant is operated, contribute significantly to the overall energy and resource efficiency. In order to influence the operational policies, reliable indicators are needed in real-time, meaning with an update rate that is compatible with the frequency of changes and the response times of the process elements.

The real-time REIs are intended to capture the current technical performance of a plant, such that they can be used to monitor and optimize the operation with respect to resource efficiency. General principles for the definition of resource and product specific REIs were described first for continuously operated processes and demonstrated for an ethylene oxide plant (Kalliski et al., 2015) and are the basis for this chapter.

2.2.1 Definitions

Large parts of this section were published in Kalliski and Engell (2017)[5] *and Beisheim et al. (2018)*[6].

Depending on the intended field of application, the interpretation of the terms "resource efficiency" and "real-time" differs. A clear understanding of these terms is necessary as a basis for the subsequent discussion.

Resource efficiency

Resource efficiency is understood as a vector of indicators that includes the environmental load and the efficiency of the utilization of different materials and carriers of energy in the production of the desired products. Other resources such as manpower, production capacity, and capital are not included in the discussion here as they are captured by the usual economic indicators.

Real-time

A measurement, analysis, or optimization technology is considered as "real-time" in the context of resource efficiency indicators if:

(1) The time delay and the sampling time of the entire analysis procedure (measurements and data processing) are sufficiently short compared to relevant process dynamics.

(2) The time resolution is similar to the typical frequency of changes of manipulated variables.

Due to the presence of disturbances and fluctuations in all production processes, REIs have to be averaged over sensible intervals to avoid that their values are affected by stochastic influences. On the other hand, the averaging must not be longer than the periods over which the manipulated variables are kept constant. Because then the effect of the operational policies would become blurred.

Plant Topology

In industrial practice, energy efficiency monitoring is mostly performed on plant or site level by relating the amount of products to the utility usage. In order to improve the efficiency, the most energy intensive processing steps are assessed to identify improvement

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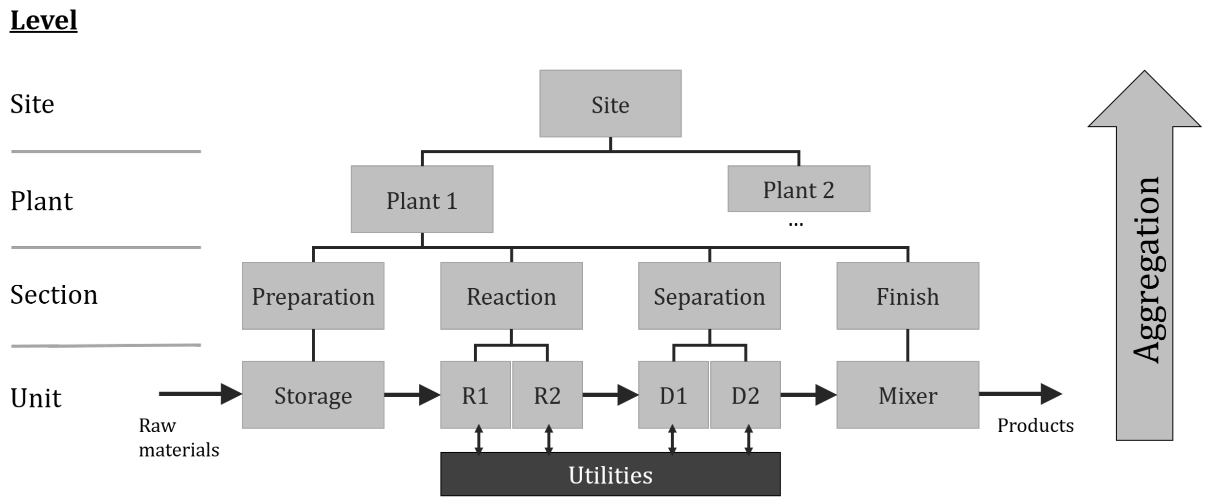

Figure 2.2: Hierarchical structure of a production site on four levels, with the reaction stages $R1$, $R2$ and the distillation stages $D1$, $D2$.

potentials. The indicator framework outlined in this chapter aims to start the assessment on the unit level, while extending it to other aspects of resource efficiency. This way it is possible to analyze the impact of operational decisions and improve the efficiency of the processing unit. The REIs serve multiple purposes on different levels of the plant hierarchy (cf. fig. 2.2). On unit level they should be used to steer the equipment towards a more efficient production, and indicators on plant or site level should serve the purpose to monitor the long term efficiency and confirm that local optimization efforts also improve the global performance. On the lower level, care must be taken that the indicators are not misleading and cause a shift of the burden from one unit to another, when the operators optimize one locally. Beisheim et al. (2020) developed an elaborate aggregation concept for REIs that assesses the average efficiency per time period on the unit level and aggregates them to plant- or site-wide performance measures. This approach is highly suitable for continuously operated production facilities that are at steady-state.

2.2.2 Principles for resource efficiency indicators

Large parts of this sections were published in Kalliski and Engell (2017)[7] *and Beisheim et al. (2018)*[8].

The following principles are the guiding foundation for the indicator framework and ensure the suitability for real-time application.

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Gate-to-gate approach
The goal is to improve the operational performance of a production site, a plant or a process unit. Thus, the balancing domain is defined and all inflows and outflows across the delimitation are evaluated. The indicators are calculated with respect to the balancing domain, thus reflecting the technical performance of the technical system. The environmental impact associated to the raw materials, energy and logistics is not considered, to be independent of business decisions on procurement and distribution. However, the method can be extended to a life cycle analysis, which estimates the complete environmental impact of a product.

Material and energy flow analysis is the core
Resource efficiency means "more from less". The resource efficiency indicators are based on the physical flows and conversions of raw materials and energy to products and emissions to the environment. All relevant inflows, outflows and environmental impacts must be captured. The material and energy balances must be closed which poses significant challenges to the measurements of flows and concentrations. If the same input material can be either converted into the desired product or serve as a source of energy, an integrated energy and material flow analysis must be performed.

Resource and output specific
In the first step, the resource efficiency should be measured with a fine granularity, i.e. for all products and inputs of material and energy separately. Product specific REIs are defined with respect to all resources used and products produced in a process as in Eq. 2.1.

$$REI_{RPS} = \frac{Product\ Output}{Resource\ Input} \tag{2.1}$$

Here, the term "product" refers to a product with specific properties (purity, colour, etc.) and different product specifications will lead to a different consumption of energy and raw materials, e.g. due to the need of more intense purification steps. Similarly, the use of different raw materials may lead to other efficiencies, which must be reflected in specific indicators. In a second step, the indicators can be aggregated for reporting purposes, or averaged over similar products and feedstock.

Normalize to the best possible operation
The value of a resource and product specific REI by itself does not show whether the process is operated well. It should therefore be related to a reference (cf. Eq. 2.2), yielding the normalized resource efficiency, which indicates how close the current operation is to a best possible case. The best-case scenario can be obtained from a theoretical analysis (based on a model) or from the best demonstrated practice (based on historical data).

$$REI_{norm,1} = \frac{REI_{RPS}}{REI_{RPS,best-case}} \tag{2.2}$$

In case a lower bound for the indicator value is known Eq. 2.3 can be used to achieve a more sensitive KPI. The lower value $REI_{RPS,min}$ can be an implicit process constraint or the minimal REI value on the Pareto front.

$$REI_{norm,2} = \frac{REI_{RPS} - REI_{RPS,min}}{REI_{RPS,best-case} - REI_{RPS,min}} \tag{2.3}$$

REIs are needed on different time-scales
In the definition of REIs the choice of the temporal aggregation interval is crucial. It must be adapted to the system's time constant and the time between decisions. Thus, a weekly assessment can be sufficient to track the efficiency deficit due to catalyst decay, but cannot capture the influence of the day-night cycle. Furthermore, the filling or depletion of internal storage must be taken into account, because it can distort the true efficiency.

Include the environmental impact
The impact on the environment must be taken into account separately to measure the ecological performance. A full Energy Flow Analysis (EFA) and Material Flow Analysis (MFA) will include energy losses and pollutant streams; however the streams of pollutants may be so small that they hardly affect the overall resource efficiency. Therefore, emissions to air, water and soil as well as the generation of solid waste should be measured by dedicated indicators. Depending on the environmental impact of the emission and the disposal method, the waste streams must be assessed separately, e.g. the emission of $\mathrm{CO_2}$ is less harmful than the equal amount of phosgene. Moreover, for reporting and assessment purposes, the REI concept can be extended to a Life Cycle Assessment (e.g. CO_2-footprint) by weighting the different streams with the upstream impacts.

Hierarchy of indicators
For the operation of a unit, the operators need local indicators that measure the performance of the unit, e.g. the amount of steam used by a distillation column. Such REIs for an individual apparatus may, however, be misleading, because resource utilization can be shifted to other units by different local operational policies. Therefore, the primary resource efficiency indicators must be defined on a scale where the net effect of the operational policies on the resource efficiency is measured in a meaningful way, e.g. the plant level. Then, secondary indicators can be introduced on the unit level, but must be related to carefully chosen specifications of the performance (e.g. a certain purity of the stream leaving a column).

Focus on technical performance independent of external economic factors
The bottom line of a plant is its economic performance to which the resource efficiency contributes significantly. However, the economic figures are strongly influenced by external factors like prices for electricity, gas and oil or revenues from the different products. These economic factors vary independent from the operational performance and therefore the resource efficiency should in the first step be measured independent of these influences. As trade-offs between the environmental and economic performance may exist, resource efficiency and profitability should in the best case be represented as a multicriterial optimization problem.

2.2.3 Indicator selection

Large parts of this section were published in Beisheim et al. (2018)[9].

After a set of possible REIs have been chosen, the following iterative evaluation process should be used:

(1) **Preselection:** Select a set of promising indicators. While a low initial number of indicators ease a subsequent comparison, they might not cover all aspects of resource efficiency. Thus, be sufficiently broad but focus on the most important aspects.

(2) **Evaluation I:** The first evaluation should be based on a formal method like a questionnaire with the aim of reducing the number of REIs that will be considered further. In this step, some basic issues should be checked. Is the indicator useful for the time horizon considered (real time)? Is it possible to influence the indicator or is it driven by external influences only? Is the required data for the computation available and of sufficient quality or are additional measurements needed? Is it realistic to assume that these measurements will be installed? Considering the process at hand, add further questions.

(3) **Implementation:** The pre-selected indicators should be implemented and fed with real process data. This can be tested offline with low initial effort and a high flexibility to check different operating conditions such as load, fouling and weather. In contrast, an online implementation will possibly show the influence of operational decisions on the REI, but induces a higher initial implementation effort.

(4) **Evaluation II:** The implementation is followed by a second evaluation, where the same questions as before are asked. Practical experience with the real process (data) will either substantiate or change the first evaluation.

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(5) **Summary and result:** In the last step, all tested REIs are compared. Check whether all relevant aspects of resource efficiency are covered and whether the indicators explaining these aspects perform well. Screen the compiled list of candidates again, bearing the shortcomings of the current set in mind (Go to step 1 if required).

An evaluation method suitable for steps 2 and 4 is the MORE RACER method (Kalliski et al., 2015) that is explained in detail in the following section.

The MORE RACER Evaluation Framework

In an annex to the impact assessment guidelines (European Commission, 2009) the European Commission listed five topics to consider while evaluating the quality of key performance indicators: Relevant, Accepted, Credible, Easy, and Robust (short RACER). Based on an adaptation in the scope of the EIPOT project (Lutter and Giljum, 2008), the MORE RACER framework is specifically developed to address the evaluation with respect to the requirements of real-time REIs (Kalliski and Engell, 2017). Below, subtopics for all RACER categories are developed to assess the REIs in detail.

- **Relevant**
  - *Goal related:* The indicator has to be related to resource efficiency and must reflect changes in the process performance.
  - *Suitable for the time horizon considered:* The indicator is suitable for real-time monitoring. The time scale considered must be suitable for the considered process, which might be minutes or hours for continuous processes and campaigns or batch times for batch processes.
  - *Influenced by the actions of the operators:* Decisions and actions applied by the operators have an influence on the REI.
  - *Transferability to other plants or processes:* REI should be applicable to other plants and processes in order to gain benefits from a unified approach.

- **Accepted**

  Stakeholder acceptance is helpful for the realization of resource efficiency monitoring and optimization projects. The REIs should be suitable for reporting and strategic decision-making.
  - *Plant managers:* Meaningful reflection of the overall process performance and indicator transparency is required.
  - *Plant operators:* Unambiguous and transparent REIs that can guide decisions support acceptance.

  - *Academia:* Concepts and indicators accepted by academia are more likely to be the subject of teaching, further research and improvement.
  - *Public:* The REIs can be used in communication to customers and to the general public.

- **Credible**
  - *Consistency in direction and magnitude:* Changes in the value of the REI occur when the actual performance in terms of resource efficiency changes. The direction of change is the same for the REI and for the real performance, and the relationship is ideally linear.
  - *Unambiguous:* Information given by an indicator is clear and can be used for decision-making without the need for extensive explanations.
  - *Transparency of data collection and data treatment:* It is explicitly stated how data should be collected and measured and which pretreatments (filtering, averaging) is applied.
  - *Avoidance of double accounting:* The REI does not describe the same phenomenon as an already utilized REI. Computation of the REI does not count an influence twice.
  - *Clear documentation of assumptions and limitations:* Assumptions that are made and limitations of the indicator are pointed out.

- **Easy**
  - *Technical feasibility:* Hardware and software to measure, calculate and display an REI are available or can be easily installed. It is technically feasible to realize an appropriate sampling rate and measurement delay for the considered time horizon.
  - *Data availability:* Measurements for required data is existent and historical data is available as a reference.
  - *Automatically compiled, displayed and reported:* It is feasible to implement an automatic processing of measurement data, such that the indicator is computed and displayed in real-time to give feedback of the current resource efficiency. Furthermore, batch or periodical reports are compiled to enable the user to impact assessments of his actions.
  - *Predictive models can be derived:* Models that represent the response of the indicators for a resource managed unit (RMU) (see Chapter 7) to the actions of the operator at the required level of detail exist or can be derived.

- **Robust**
  - *Theoretical background:* The theory behind the definition of the indicator is valid without gaps or assumptions.
  - *Data quality:* The accuracy and reproducibility of the (processed) measurements is good enough such that the indicator does not fluctuate considerably.
  - *Reliability:* Measured values are of good precision with little error and a consistency check is possible.
  - *System boundaries, energy and mass balances:* Balances of the system in terms of energy and material can be closed, with a clear definition of the system boundary. There is no missing information on important streams.

Application of the RACER Framework

The adapted RACER framework is practically applied in the following way: A grading system for all the main criteria and their sub-criteria presented with a scoring range between zero and two points is used. Zero points means "criterion not fulfilled", one point means "partially fulfilled" and two points mean "completely fulfilled" (Lutter and Giljum, 2008). In addition, keywords should be used to annotate the scoring for subsequent revisions and possible enhancements of the indicator. During the rating, scores are assigned to all sub-criteria. The averaged values are the scores for the five main criteria. Some sub-criteria can be classified as knock-out criteria. If they are given zero points, they override the other criteria and the main criterion also receives zero points. An example would be the sub-criterion "goal related" of the category "Relevant": An indicator which does not fulfill this criterion cannot be relevant as an REI, irrespective of the remaining sub-criteria. The scores of the main criteria are visualized in a radar chart to provide an overview that can also be used to quickly compare different indicators. Fig. 2.3 shows a typical result: The RACER scores of three arbitrary REIs that were supposed to represent a similar aspect of resource efficiency are shown. It can be seen that the first indicator (REI_1) is not suitable, although the credibility looks promising. Comparing the other two indicators reveals that the second REI is worse than the third, except in the category "Robust". Therefore, REI_3 would be selected.

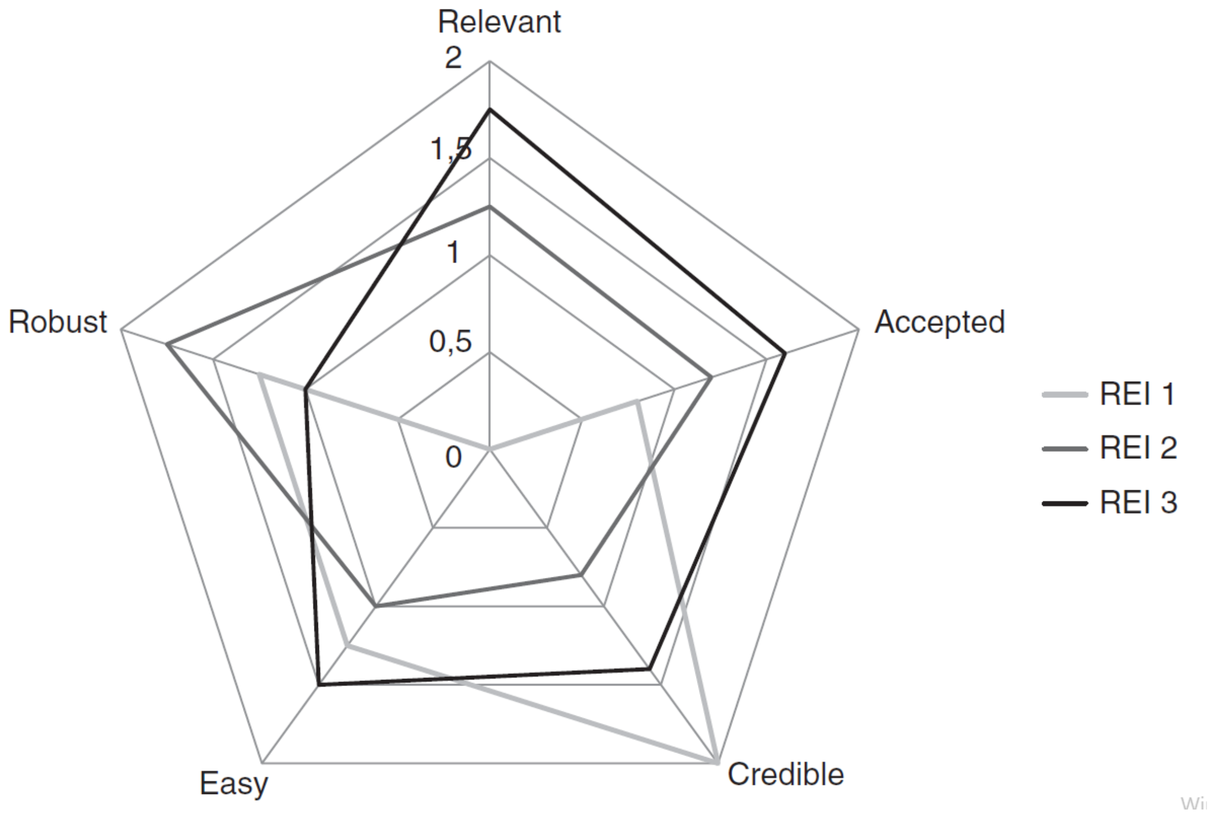

Figure 2.3: Evaluation of proposed REI using the RACER framework.

Chapter 3

Resource efficiency indicators for batch processing plants

Large parts of sections 3.1–3.4 have been published in Kalliski and Engell (2017)[1] *and Beisheim et al. (2018)*[2]*. The application case 3.5 was published in Kalliski and Engell (2017)*[1] *and it's model was adapted from a previous work of Reinaldo Hernandez. The simulation study was performed by the intern Cristhian Oliveira under guidance of the author Marc Kalliski.*

This chapter extends the methodology in section 2.2 to production processes that are completely or partially performed in discontinuous (batch or semi-batch) operation mode. These processes account for a significant share of the total production volume of chemical plants and are widespread in the production of specialty chemicals, polymers, food and drinks, and pharmaceutical ingredients (Cefic 2014). The tracking of the resource efficiency in batch processes requires additional considerations regarding the allocation of resources to specific batches and the impact of production logistics on the overall efficiency of the process. In section 3.5 the presented framework for the definition and utilization of real-time batch REI is applied to the case study of a sugar plant that incorporates discontinuous and continuous production stages. The plant model was taken from Mazaeda et al. (2014) and is extended by resource efficiency considerations in the scope of this thesis.

3.1 Monitoring of batch efficiency

This section has been published in Kalliski and Engell (2017)[1] *and Beisheim et al. (2018)*[2]*.*

Batch processes are dynamic in nature and require the tracking of the batches to ensure the correct allocation of the used resources to the individual batches. Thus, the data collection and calculation of REIs require modifications compared to the continuous production. Effects that have an influence on the overall resource efficiency occur on different temporal and hierarchical levels, and specifically designed REIs help to capture the influences on the resource efficiency on all levels (process unit, plant, site).

The evolution of the indicators during the production steps of a batch (e.g. a reaction step) can be used to assess the distance to a known optimal trajectory, but only after the completion of the batch the overall resource efficiency can be determined. In order to determine the resource efficiency of the production of a single batch, the resource utilization must be measured with a sufficiently fine resolution so that the resources can be attributed to the individual batches.

Many operational aspects that may have an influence on the resource efficiency of batch production plants, such as the sequencing and scheduling of the unit operations, can only be assessed for a larger number of batches. Therefore, in addition to indicators for the single batch, global indicators of the efficiency of the plant over many batches (e.g. production campaigns) are needed. On the plant-wide level it is also possible to identify slow dynamics that call for optimization (e.g. catalyst deterioration).

For crucial processing steps, local indicators can be defined to help the operating staff to assess the efficiency of the individual production stages. However, since performing a reaction longer to reach a higher conversion may save energy in subsequent separation steps, a full assessment is only possible at the end of the production sequence.

Resource efficiency indicators for batch processes will usually be strongly dependent on the product specification (e.g. product purity, optical properties) and may also depend on the size of the batch for the same product. Whether or not they can be aggregated over several products depends on the specific situation. The batch duration and the lot sizing are degrees of freedom that can be exploited during the optimization of the process.

Batch Resource Efficiency

As stated above all used resources are recorded individually and related to the amount of the resulting product. Figure 3.1 shows the typically occurring streams crossing the system boundary of the batch where m_k is the mass of raw material k fed to the batch, $Q_{H,i}$ is a heating energy, $W_{el,i}$ is electrical energy consumed, $Q_{C,i}$ is cooling duty, m_{waste} is the material that is discharged from the process, $m_{product}$ is the product material obtained during the batch, $W_{generated,j}$ is the electrical energy obtained from the batch that is consumed elsewhere, and $Q_{generated,j}$ is the energy that is discharged from the batch and used elsewhere.

In case excess heat or electricity is generated during the production and used in another unit, the resource consumption needs to be corrected according to Equation 3.1:

$$REI = \frac{Product\ Output}{Resource\ Consumption - Resource\ generated} \tag{3.1}$$

This is initially done for each resource separately. If desired, aggregated indicators for the total energy or material efficiency can be derived from the resource and product specific sets of indicators. Contrary to the definition above, the indicators can also be defined inversely, as intensities, to facilitate interpretation in connection with the naming of the indicators.

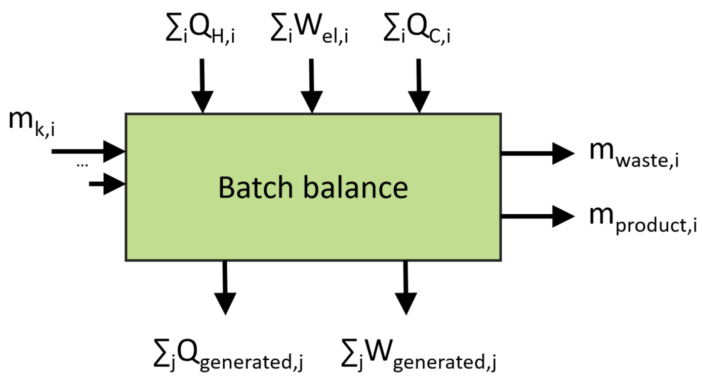

Figure 3.1: Simplified batch balance.

Energy efficiency

The energy efficiency is an important factor, because of the associated costs and environmental impact. For the electrical energy efficiency (EEE, Equation 3.2) the product mass is related to the electrical energy consumption of pumps, motors, and other consumers in the production line:

$$EEE = \frac{m_{product}}{\sum_i W_{el,i} - \sum_j W_{gen,j}} \tag{3.2}$$

The heating energy efficiency (HEE, Equation 3.3) and the cooling energy efficiency (CEE, Equation 3.4) are defined in order to evaluate the energetic performance of the batch. They are correlated to the material efficiency in cases when reaction rates are a function of temperature. Hence, there can be a trade-off between the energy and the material efficiency:

$$HEE = \frac{m_{product}}{\sum_i Q_{H,i} - \sum_j Q_{gen,j}} \tag{3.3}$$

$$CEE = \frac{m_{product}}{\sum_m Q_{C,m}} \tag{3.4}$$

The CEE is generally expressed with reference to the cooling duty, but if the coolant is prepared within the balance area it can be substituted by the utility imported to generate it. Mostly air, water or other liquid agents are used as coolant, but not altered or consumed with the exception of an increased discharge temperature. Finally, the aggregation to the total energy efficiency (TEE) is defined in Equation 3.5:

$$TEE = \left(\frac{1}{CEE} + \frac{1}{HEE} + \frac{1}{EEE}\right)^{-1} = \frac{m_{product}}{\sum_i W_{el,i} + \sum_j Q_{H,j} + \sum_m Q_{C,m} - \sum_n Q_{gen,n} - \sum_t W_{gen,t}} \tag{3.5}$$

Sometimes, during chemical reactions or physical state changes that are taking place within the process, heat is emitted. In case the generated heat can be used elsewhere in the plant, it is not counted as waste heat (causing cooling effort) but as a heat product HP (Equation 3.6):

$$HP = \frac{\sum_i Q_{gen,i}}{m_{product}} \tag{3.6}$$

Material efficiency

The material input intensity (MI_k, Equation 3.7) is defined as the amount of raw material k used divided by the mass of the total product obtained by the batch under investigation. If the process is efficient, more product is obtained from the same amount of raw material, thus MI_k decreases, wherein $m_{in,k}$ is the amount of k introduced to the batch:

$$MI_k = \frac{m_{in,k}}{m_{product}} \tag{3.7}$$

For an overview of the material efficiency in the case of multiple raw materials, the total material efficiency (TME, Equation 3.8) is introduced. Here, the product mass is related to the total raw material consumption.

$$TME = \frac{m_{product}}{\sum_k m_{in,k}} \tag{3.8}$$

The material efficiency (ME_k, Equation 3.9) of raw material k is defined as follows:

$$ME_k = \frac{\sum_p m_{k,stoic,p}}{m_{in,k}} \tag{3.9}$$

$m_{k,stoic,p}$ is the mass of reactant k that is incorporated into valuable product and $m_{in,k}$ is the mass of substance k fed to the batch. The material efficiency improves with the selectivity of the reaction $\left(\sum_p m_{k,stoic,p} \text{ increases}\right)$ and the minimization of raw material input ($m_{in,k}$ decreases). For an arbitrary reaction according to Equation 3.10, $m_{k,stoic,p}$ is calculated by Equation 3.12. The required coefficients $n_{k,p}$ are obtained by decomposition into the ideal net formation reactions of the products (see Equation 3.11):

$$\underbrace{\sum_k \nu_k R_k}_{\text{reactants}} \rightarrow \underbrace{\sum_p \nu_p P_p}_{\text{products}} + \underbrace{\sum_t \nu_t W_t}_{\text{waste}} \tag{3.10}$$

$$\sum_k \nu_{k,p} R_k \rightarrow \nu_p P_p \qquad \forall p \;\; \text{with} \;\; \nu_k = \sum_p \nu_{k,p} \tag{3.11}$$

$$m_{k,stoic,p} = n_{k,stoic,p} M_k = n_p \frac{|\nu_{k,p}|}{\nu_p} = m_p \frac{|\nu_{k,p}|}{\nu_p} \cdot \frac{M_k}{M_p} \quad \forall k, p \tag{3.12}$$

Here, M_k and M_p are the molecular weights and $\nu_{k,p}$ and ν_p are the stoichiometric coefficients. In cases where the raw material is converted to multiple products or to an additional undesired side product, the atom efficiency is taken into account.

There are two different possibilities to define the amount of product used for the calculation of the resource efficiency indicators, the first being the total amount of formulated product within the specification including additives or remaining solvents, the second being the net product contained in the final formulation. Using the first definition of product material, the concentration of the valuable component can be optimized, but the sensitivity to the material efficiency is lost for highly diluted products. In the second case, the indicators are always sensitive to the chemical/material efficiency, but the dilution of the valuable component is not taken into account, hence it is not possible to minimize the concentration of the valuable component within the product specifications to avoid over-purification. To illustrate the effect, three cases are compared in Figure 3.2 that are based on the reaction in Equation 3.13.

$$\text{Reaction equation: } R \rightarrow P \tag{3.13}$$

The solvent water is considered to be inert in the reaction and the product is specified to contain up to 80% water of which a part may simply be added in the final production stage. At the same time only 20% of the raw materials end up in the product, resulting in a total material efficiency of 55.6% (case 1), despite the fact that the efficiency of the chemical conversion is poor. Changing the formulation to contain 85% water increases the resource efficiency to 62.5% (case 2) but in fact nothing has changed except that more water has been added to the product.

The same increase would be obtained by an increased yield of 25% (case 3). In one case, the loss of material R is $4kg$ of raw materials per kg of product P. In the latter it is only $3kg$ per kg of product P, but due to the dilution, the two processes seem to be similarly efficient. In addition, the dilution improves the environmental indicators except of the use of water. Hence, when different product formulations are compared, the net amount of valuable product should be used as a basis. The material efficiency per valuable product is also more sensitive to changes in the operation of the process.

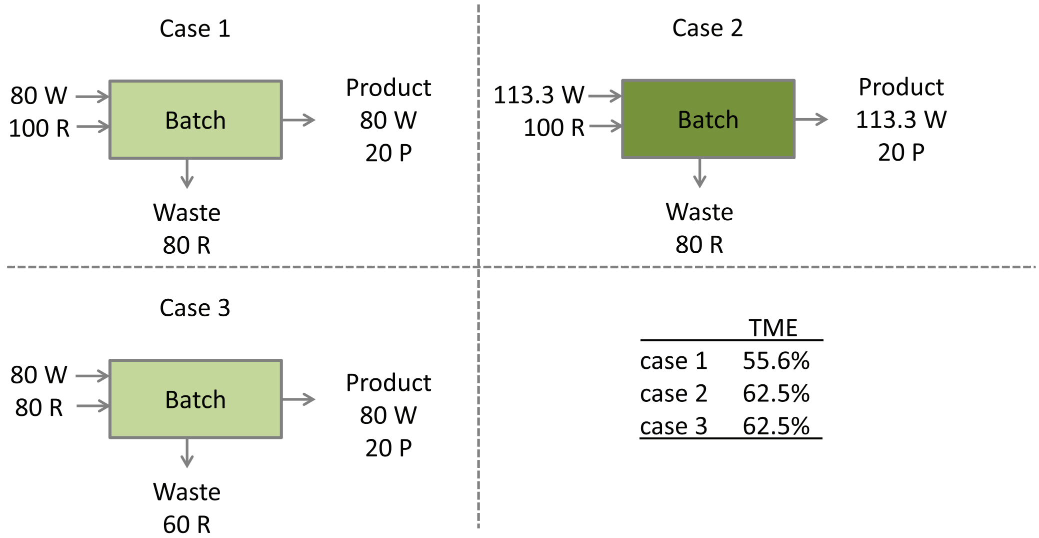

Figure 3.2: Example for the total material efficiency (TME).

Water and waste efficiency

Another factor in the context of resource efficiency is the environmental impact that is caused by industrial processes. Besides the resource intake that is covered by the REIs above, processes also emit waste streams. The compounds contained may have a negative impact on the environment and thus need to be monitored as well, in the form of the waste production indicator WP_j for all j components occurring in the process (Equation 3.14). Wherein, $m_{waste,j}$ is the total amount of component j contained in waste streams:

$$WP_j = \frac{m_{waste,j}}{m_{product}} \tag{3.14}$$

The total mass-based waste production (TWP, Equation 3.15) is then defined as the sum over all WP_j:

$$TWP = \frac{\sum_j m_{waste,j}}{m_{product}} \tag{3.15}$$

Additionally, water is often consumed in industrial processes or polluted with chemical residues. Since water is often a scarce resource, the water usage per product (WU, Equation 3.16) is an important indicator of the environmental burden:

$$WU = \frac{m_{water,in}}{m_{product}} \tag{3.16}$$

It might be necessary to define additional indicators to describe other environmental impacts associated with the process. These indicators vary from case to case and have to be tailored individually.

REIs for key production phases

The production phases involved in the processing of a batch are defined in recipes that contain the allocation of operations to units, the type of consumed materials, the procedures for purification, and the sequence of production phases to be executed (see Figure 3.3). The timing and equipment allocation for each execution of the batch recipe result from a scheduling process that takes into account the number, types, and sizes of the batches that have to be produced, sequencing constraints, and allocation constraints.

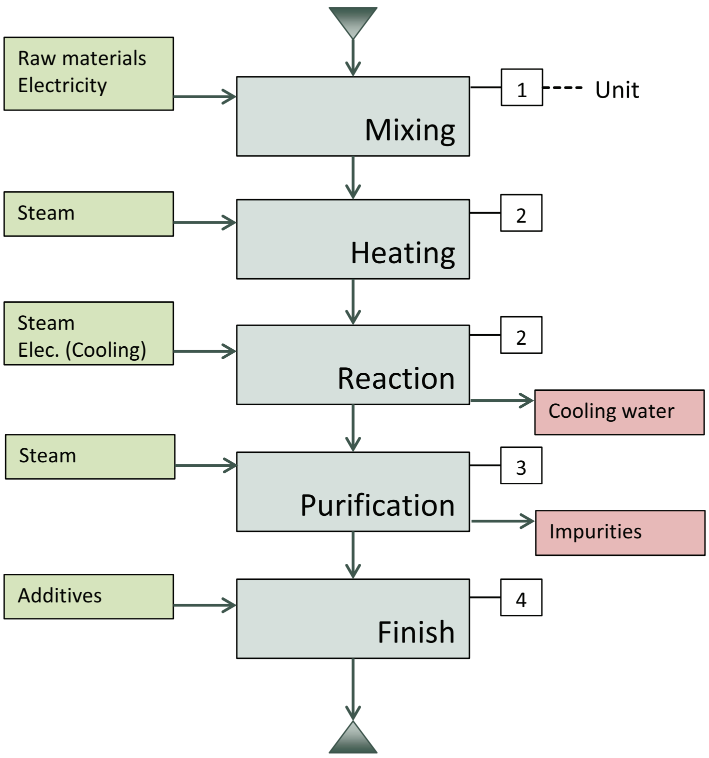

Figure 3.3: Batch recipe example.

The most energy-intensive phases are the reaction and purification phases, due to the enthalpy of reaction and the enthalpy of evaporation. Furthermore, the yield and conversion of the reaction as well as the amount of losses during purification are strongly affecting the material efficiency. Thus, local indicators that are specifically monitoring these production phases are defined below and can be useful to improve the efficiency during daily operations if visualized to the operating staff.

Reaction efficiency

The efficiency of the chemical reactions involved in the production process determines the overall material efficiency to a large extent. An efficient reaction is accomplished when all participating reactants are converted to the desired products according to the chemical stoichiometry. The reaction efficiency (RE_k) of participating species k is defined analog to the material efficiency (ME_k), but here only the mass of raw material k in the reaction stage is considered. Thus, losses of reactants or product due to inefficient purification steps before or after the reaction are not included. Hence, the reactant efficiency (RE_k) of the participating species k is defined as:

$$RE_k = \frac{\sum_p m_{k,stoic,p}}{m_{feed,k}} \tag{3.17}$$

$m_{feed,k}$ stands for the amount of reactant k that was charged into the reactor before and during the course of reaction. $m_{k,stoic,p}$ is the mass of reactant k that was incorporated in the product. If species k is a reactant for more than one product component, then the sum over all shares of k in the products p has to be used.

Analogous, the total reactant efficiency (TRE) over all reactants is derived:

$$TRE = \sum_k \frac{\sum_p m_{k,stoic,p}}{m_{feed,k}} \tag{3.18}$$

These indicators show the reaction efficiency on an easily comprehensible scale from 0 to 100%.

Purification efficiency

Purification operations are used to remove undesired components from the mixture of materials that are fed to the process or that result from reaction steps. This can for example be necessary for raw materials from natural resources that contain catalyst poison and for product materials that contain undesired byproducts, unreacted raw materials, catalyst, or solvents. The information about the resources used in the separation stage and the amounts and compositions of the output streams are sufficient to calculate the corresponding indicators.

In the example shown in Figure 3.4 a mixture of reactant A, valuable component C, and water W obtained from a prior reaction stage is fed to the purification stage. A batch distillation is conducted to remove the unreacted feed A and an excess of water. The residual of C and W form the product and the product is in specification if:

a) the concentration of C in the product mixture is above the purity limit and

b) the contamination with A is below the contamination limit.

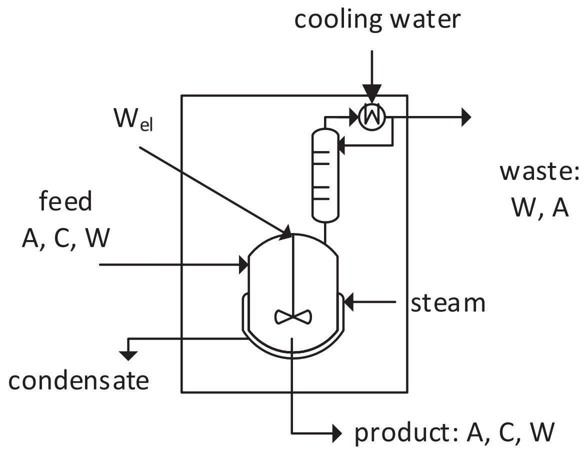

Figure 3.4: Batch distillation with removal of raw material residue A and excess water W.

The efficiency is at its maximum if the separation yield SY_{CW} is at its maximum (see Equation 3.19).

$$SY_{CW} = \frac{m_{resid,C} + m_{resid,W}}{m_{feed,C} + m_{max,resid,W}} \quad \text{s.t.} \quad m_{resid,W} \leq m_{max,resid,W} \tag{3.19}$$

The highest SY_{CW} is obtained when the entire amount of valuable C remains in the product mixture, resulting in SY_{CW} being equal to 1 (or 100%) and $m_{resid,W} = m_{max,resid,W}$. This way the SY_{CW} solely reflects the separation performance. The resource efficiency of the purification step is mostly affected by the amount of energy consumed. Here, the electrical energy (W_{el}) consumed by the stirrer motor, the cooling duty (Q_C), and the heating energy (Q_H) by steam are contributing factors to the purification energy efficiency (PEE, see Equation 3.20).

$$PEE = \frac{m_{product}}{Q_H + W_{el} + Q_C} \tag{3.20}$$

In most cases the separation yield and the purification energy efficiency will be competing objectives, as longer distillation times lead to a higher product purity (improving SY_{CW}) but also to a larger energy demand (worse PEE). The optimal operation must be determined on the basis of plant-wide REI. The resulting optimal values for the SY_{CW} and PEE are then used to locally operate the purification.

3.2 Plant-wide contributions to resource efficiency

This section has been published in Kalliski and Engell (2017)[3] *and Beisheim et al. (2018)*[4].

The indicators that were presented in the previous sections measure the resource efficiency for a single batch. In addition to the feed of raw materials and energy that is directly related to one batch, other contributions may occur on longer time scales, e.g. the replacement of catalyst, the treatment of material in a recycle, and cleaning operations. It is not adequate to associate the resource consumption of these operations only to the batches that are performed immediately before or after the operation. To overcome this issue, a large number of batches are considered, with multiple occurrences of the long term effects, resulting in the overall resource efficiency (ORE). Equation 3.21 defines ORE_{cat} to capture the resource efficiency associated with catalyst utilization:

$$ORE_{cat} = \frac{\sum_b m_{total,product,b}}{\sum_b m_{cat,makeup,b}} \tag{3.21}$$

All contributions are added up for a suitable number of batches b, to arrive at meaningful values. Similarly, the ORE_{clean} can be defined where $m_{cleaning}$ is the total amount of cleaning agent used for cleaning and $m_{product,b}$ is the mass of product obtained in batch b (see Equation 3.22).

$$ORE_{clean} = \frac{\sum_b m_{product,b}}{\sum_b m_{cleaning,b}} \tag{3.22}$$

If referenced against the best achieved practice, the ORE can indicate a poor performance due to the long-term effects on resource efficiency. The reasons for a possible loss of efficiency can be investigated by comparison of the operating conditions during the best-demonstrated practice and the current set of batches. Plant-wide logistics (production planning and scheduling) are an important influencing factor for the overall resource efficiency (ORE), because the sequencing and allocation of operations and batches may lead to additional unnecessary resource consumption. For example, at an intermediate stage the batches may need an elevated temperature level to prevent the formation of solids. In case of bad timing and long waiting periods, the energy consumption increases. In the case where bad scheduling results in products or intermediates that are off-spec, a rework may be necessary, further increasing the consumption of resources. The aggregation interval must be chosen long enough to show the effect of scheduling decisions adequately.

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Figure 3.5 shows the influence of the scheduling on the amount of utilized resources caused by sequence-dependent changeovers. Two dispatching strategies are shown for the production of one batch of "dark", one batch of "medium", and one batch of "light" colored material. Assuming that a more intense cleaning operation takes more time and cleaning

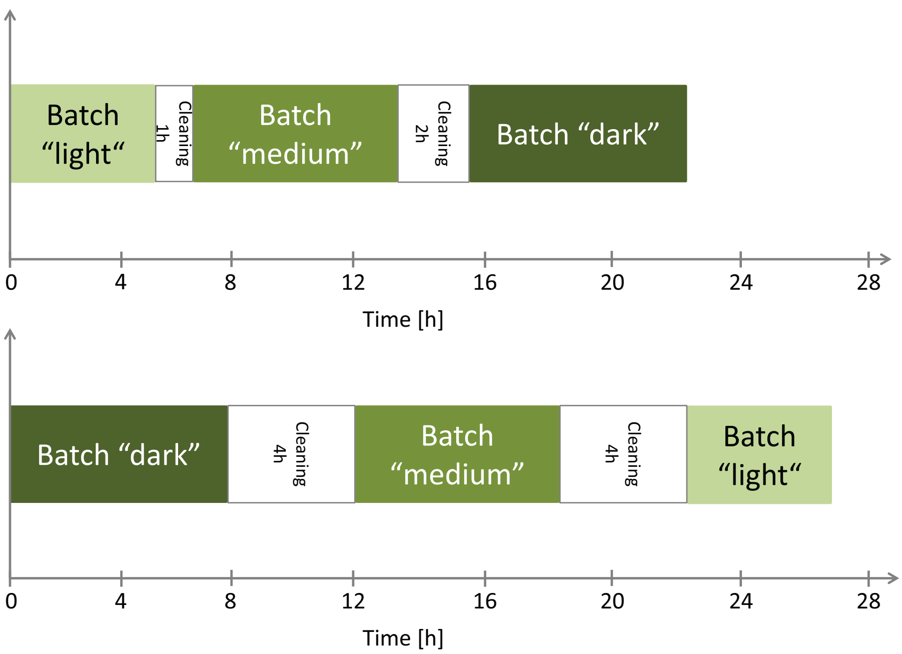

Figure 3.5: Two different schedules of the same product mix.

agent, the resource efficiency deteriorates for higher cleaning efforts. With sequence-dependent cleaning procedures, alternative sequences have a direct impact on the time and amount of cleaning agent. It can be easily seen that the required amount of cleaning agent in the upper schedule is 62.5% less than the amount required for the second one.

In case recycles occur, accumulated inert compounds and side products need to be removed periodically to reduce the negative impact on the reaction kinetics and reduce the amount of recycled material. If the purification is not performed after each batch, it is not meaningful to assign the consumption to individual batches. Thus, the purification task creates an additional waste stream and additional energy consumption that must be distributed over multiple batches on a longer time horizon (Equations 3.23-3.24).

$$ORE_{recycle,waste} = \frac{\sum_b m_{product,b}}{\sum_b m_{recycle,waste,b}} \tag{3.23}$$

$$ORE_{recycle,energy} = \frac{\sum_b m_{product,b}}{\sum_b Q_{recycle,b}} \tag{3.24}$$

3.3 Propagation of REIs

This section has been published in Kalliski and Engell (2017)[5] *and Beisheim et al. (2018)*[6].

Locally recorded indicators capture the efficiency of individual plant sections, but do not reflect the overall efficiency of the process. To measure the efficiency of the overall process, it is necessary to combine the locally recorded indicators into an overall indicator. This can be done in two ways, as shown in figure 3.6. Using the propagation approach, the material is tracked on its way through the plant and the consumed resources are recorded on a batch-specific basis. Vertical aggregation is carried out according to the plant structure, whereby the performance for individual plant sections is determined quasi-continuously and aggregated to the overall plant performance.

The vertical aggregation of local unit specific REIs that were obtained over longer periods deliver an indication on the mean performance for the overall process with low granularity. Hence, vertical aggregation is an option to report the overall efficiency over longer time horizons, e.g. a year. Batch processes can be complex and they exhibit more degrees of freedom like the production scheduling, processing times, and they also include the possibility to perform processing steps in alternative equipment. Thus, it is necessary to track the processing of materials more closely in batch facilities to track the resource efficiency with higher granularity with respect to time and location. This thesis proposes a propagation concept to track the material through the process and allocate the consumed resources to the batch that is currently processed in each unit. Thus, local REIs are obtained for each of the unit operations as resource load per mass of intermediate product and propagated. This procedure is complicated by recycle streams and the splitting or combining of product-yielding batches.

Recycled materials

In the above definitions it is assumed that all the material that enters the production of a single batch either ends in the product or leaves the process as waste. Often, however, material is recycled, e.g. solvents, raw materials, or catalysts are removed from the batch and recycled to a subsequent batch. While this material strictly speaking is “lost” for the specific batch under consideration, it is “gained” in the production of the next batches (see fig. 3.7). Considering a single batch, the introduced and recovered recycle streams should not be regarded as raw material and waste stream, because the material is effectively not lost and the indicators would give a wrong indication if this fact was not taken into account. Thus, the material efficiency for batches that include a recycling of some process

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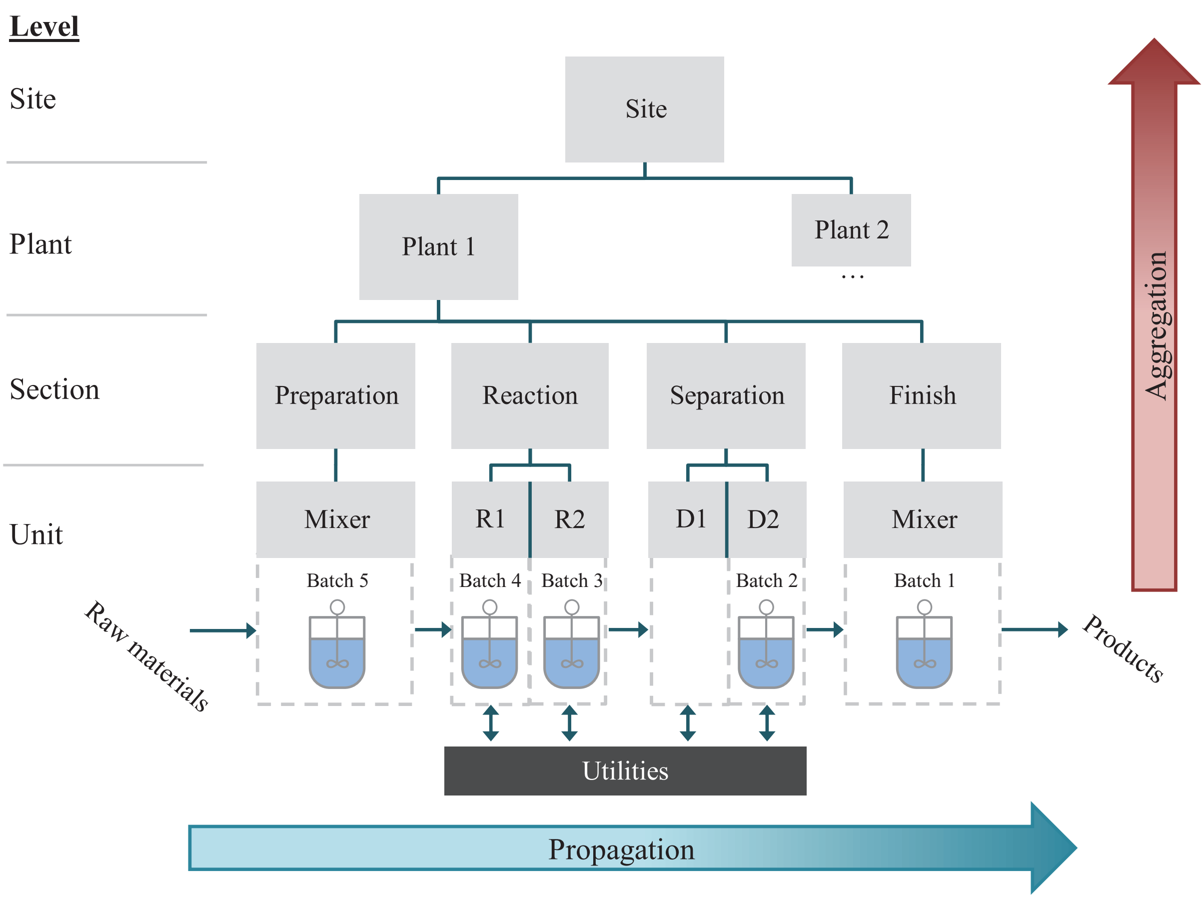

Figure 3.6: Hierarchical structure of a production site on four levels, with the reaction stages $R1$, $R2$ and the distillation stages $D1$, $D2$.

stream $ME_{recycle,k}$ is defined in Equation 3.25.

$$ME_{recycle,k} = \frac{\sum_p m_{k,stoic,p}}{m_{in,k} + (m_{in,recycle,k} - m_{out,recycle,k})} \tag{3.25}$$

With this definition the true material efficiency of raw material k for the current batch is reflected. Ideally, the amount of k in the incoming recycle is equal to the outgoing and the correction term $(m_{in,recycle,k} - m_{out,recycle,k})$ equals zero. In reality, it is likely that

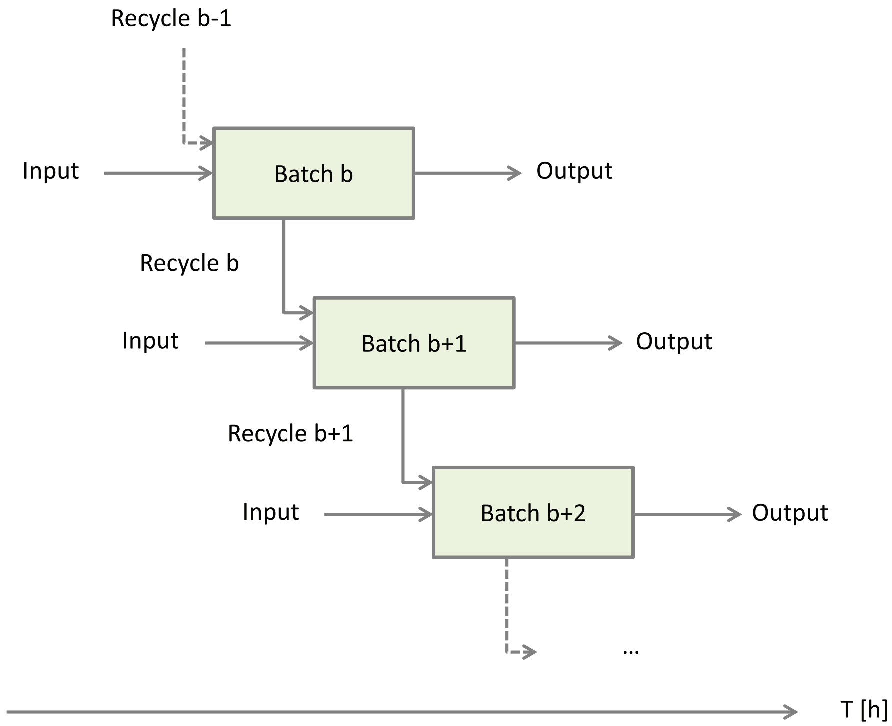

Figure 3.7: Recycle flow from batch to batch.

inert materials or side products accumulate in the recycle, calling for a purification of the recycled material. If this is happening in each batch cycle this has to be taken into account as an additional resource feed for the product batch. If the purification is performed for the recycled material of several batches, it has to be considered on the plant level within an ORE.

Uniting and Splitting of Batches

Modern discontinuously operated production sites are usually designed to produce a multitude of products with individual recipes. In batch production, a process structure as shown in Figure 3.8 can occur where two batches are processed independently from each other and are later combined to a batch of product. First, raw material A is dissolved in water under stirring. The solution then undergoes the endothermic reaction 2, requiring the heat input $Q_{H,2}$. In parallel, raw material B is converted to an intermediate I_1. This is mixed with the intermediate solution I_2 and fed to the final reaction 3. The resource efficiency calculation is similar to the case of a linear process structure, if calculated for the entire batch with the dashed line as system boundary.

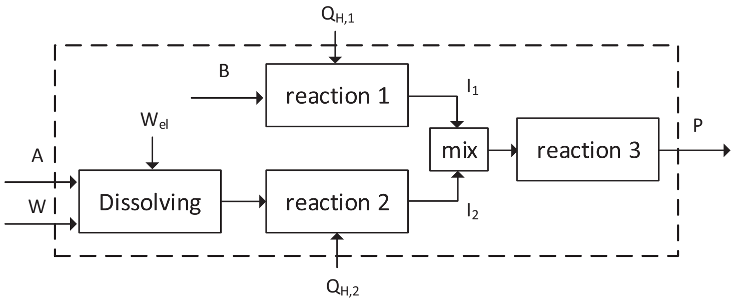

Figure 3.8: Process structure with parallel production of two intermediates that are merged to the final batch.

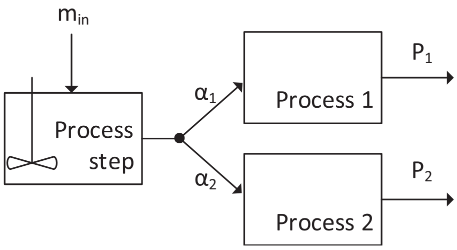

Figure 3.9: Process for two recipes based on homogeneous splitting.

Other multi-product plants are designed to produce a set of similar products that share the same basic formulation but vary in the remainder of the recipe. Here, the first processing steps are performed in large batches which then subsequently are split into smaller batches that are processed individually according to different recipes (see Figure 3.9). To compute the efficiency of the created batches, the energy and mass inputs in the stage before the split are multiplied with the corresponding splitting factor α_i in order to obtain the share of resource consumption that is related to product P_i. The splitting factor α_i (Equation 3.26) indicates how much of the initial amount (m_{in}) is used for the production of product i (m_i):

$$\alpha_i = \frac{m_i}{m_{in}} \quad \text{with} \quad \sum_i \alpha_i = 1 \tag{3.26}$$

Thus, the previously defined REI can be used in this case in a straightforward manner by weighting the energy and material consumption before the splitting operation by α_i. If the batch material is split by a separation process, it is not possible anymore to assume the same concentration in all resulting batches and thus the resources that were consumed before the separation process need to be divided by the mass ratio of desired products in the batches. An example for such a situation is shown in Figure 3.10 for a membrane separation.

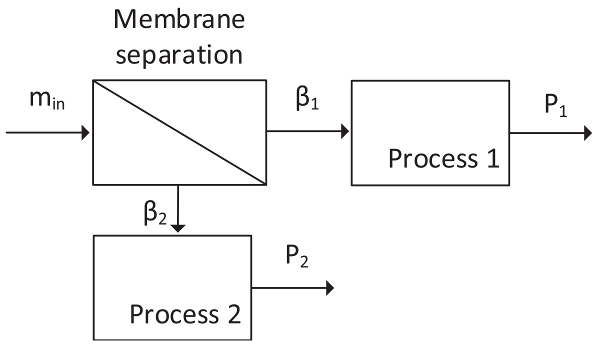

Figure 3.10: Membrane separation process, where both phases are yielding a product.

The split factor β_i is defined in Equation 3.27 for separation processes for which both phases are further processed to yield valuable products.

$$\beta_i = \frac{m_{Pi}}{\sum_i m_{Pi}} \quad \text{with} \quad \sum_i \beta_i = 1 \tag{3.27}$$

During the upstream processing that yielded the material input m_{in}, energy and raw materials were fed. This resource intake has to be distributed among the sub-batches. The energy input is attributed to the sub-batches with the help of the splitting factor β_i:

$$W_{el,i} = W_{el,in} \cdot \beta_i \tag{3.28}$$

The distribution of the raw materials is not as straightforward, since the resource efficiency indicators relate the obtained products to the raw materials that are introduced to the process. If the initial mixture fed to the separation stage contains multiple valuable products that are separated by the membrane, each raw material might have been consumed in the formation of the products to a different extent. The amount of unreacted raw materials, which is not contained in any product material, also needs to be distributed among both batches. This is done according to the ratio $\gamma_{k,i}$ (Equation 3.29) of the material equivalent of substance k in batch i per total equivalents of k in the products p. Then the amount $m_{k,in,i}$ of all materials k is attributed to the subsequent batches according to Equation 3.30:

$$\gamma_{k,i} = \frac{\beta_i \cdot \sum_p m_{k,stoic,p}}{\sum_i \left(\beta_i \cdot \sum_p m_{k,stoic,p}\right)} \quad \text{with} \quad \sum_i \gamma_{k,i} = 1 \tag{3.29}$$

$$m_{k,in,i} = \beta_i \cdot \sum_p m_{k,stoic,p} + \gamma_{k,i} \left(m_{k,in} - \sum_p m_{k,stoic,p} \right) \tag{3.30}$$

The amount $m_{k,stoic,p}$ denotes the amount of material k that was consumed during the formation of product p and is obtained from Equation 3.12.

3.4 Monitoring of mixed batch-continuous plants

This section has been published in Kalliski and Engell (2017)[7] *and Beisheim et al. (2018)*[8].

Mixed production processes contain batch-wise and continuously operated sections. When there is a transfer between the two operating regimes, special care must be taken to accurately track the resource efficiency during the material transfer, because back mixing might occur, which affects the performance. Batch and continuous sections are usually connected by buffer tanks. Variations in lot sizing, batch efficiency, and batch arrival times constantly change the states of the buffer tank. The dynamics of the mixing process are taken into account by introducing efficiency state variables to track the already consumed amount of resources per amount of product.

Transition from batch to continuous production

In the transition from batch to continuous operation, the material is usually buffered to ensure a constant transfer into the continuously operated section. The buffer tank is assumed to be ideally mixed (see Figure 3.11, left). Thus the concentrations c_i of the outlet stream $\dot{m}_{out}$ are equal to the current concentration within the tank.

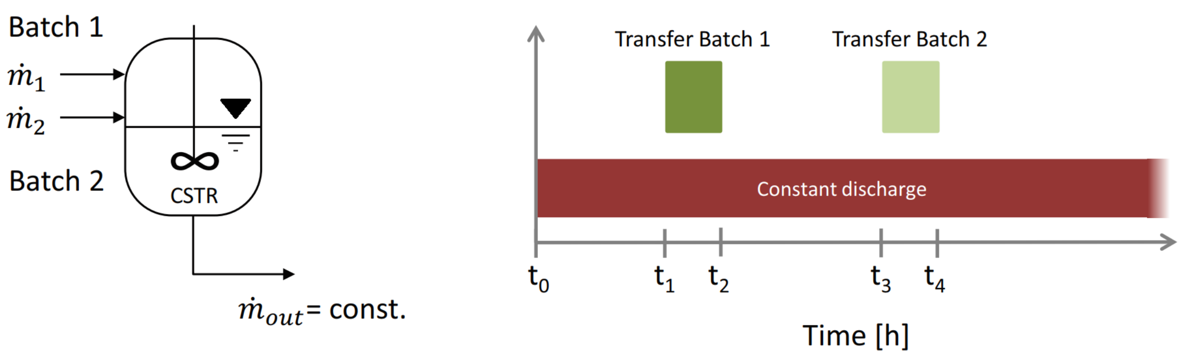

Figure 3.11: Buffer tank between batch and continuously operated section (left), timing of transfer operations to and from buffer tank (right).

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Figure 3.11 (right) shows a sequence of two batches that are fed into the buffer tank. Each batch has a known size and the transfer interval is determined by the inlet flow rate. The composition of the arriving material and the amount of resources per unit mass that were needed to produce it may vary from batch to batch. Let $r_{i,in,n}$ be the entire upstream consumption of a resource i per mass of product in batch n, and let m_p be the mass of product in the buffer tank. $r_{i,in,n}$ and the mass fraction w_n of the product in batch n vary from batch to batch, where w_n relates the amount of product that is contained in the batch to the total mass of the batch. The buffer tank can be modeled as a system of three differential equations 3.31-3.32 and 3.34 describing the states: total mass m, amount of product in the tank m_p, and specific resource utilization r_k of the resource k per amount of product.

$$\frac{dm}{dt} = \left(\sum_n \dot{m}_n\right) - \dot{m}_{out} \tag{3.31}$$

$$\frac{dm_p}{dt} = \left(\sum_n \dot{m}_n w_n\right) - \dot{m}_{out} \cdot \frac{m_p}{m} \tag{3.32}$$

The resource consumption that is “carried” by an element of product material is introduced as an additional state variable. The differential equation for a product-specific resource utilization r_k can then be derived from the balance for the resource consumption state m_{cons}:

$$\frac{dm_{cons}}{dt} = \frac{d\left(m_p r_k\right)}{dt} = r_k \cdot \frac{dm_p}{dt} + m_p \cdot \frac{dr_k}{dt} \tag{3.33}$$

Substitution of Equation 3.32 into 3.33 and solving for $\frac{dr_k}{dt}$ yields Equation 3.34.

$$\frac{dr_k}{dt} = \sum_n \frac{\dot{m}_n w_n}{m_p}\left(r_{k,in,n} - r_k\right) \tag{3.34}$$

The inlet flow rates $\dot{m}_n$ are assumed to be constant and are defined by total amount mn and the arrival times $t_{start,n}$ and $t_{end,n}$ (see Equation 3.35).

$$\dot{m}_n(t) = \begin{cases} 0, & t < t_{start,n} \\ m_n / \left(t_{end,n} - t_{start,n}\right), & t_{start,n} \leq t \leq t_{end,n} \\ 0, & t > t_{end,n} \end{cases} \tag{3.35}$$

For the example described in Figure 3.11, the trajectories shown in Figure 3.12 were obtained. Initially, the tank contains $60kg$ of product at a total mass of $130kg$ and there is a constant outflow of $2kg/min$. The initial state of the resource load r_k is 5 resource units per kg of product contained in the storage tank. In the first scenario (blue), the first arriving batch has a total mass of $60kg$ (thereof $36kg$ product), has a high resource load (24 resource units per kg of product), and is transferred into the buffer tank within $2min$

(fast). Subsequently, a second batch ($37.5kg$, $11.25kg$ product) with a resource load of 6 is transferred into the tank over a period of $10min$ (slow). In the second scenario (red), the same batches are introduced into the buffer tank with different transfer times (slow-fast). Under the assumption that the buffer tank is ideally mixed, the resource efficiency of the constant outflow is characterized by the current state r_k. Thus it is possible to propagate the resource efficiency of the batch material to the continuous outflow.

Transition from Continuous to Batch Production

In case of the transition from a continuous section into batch operation, the total resource consumption associated with the new batch n can be computed by the integral shown in Equation 3.36:

$$r_{k,n} = \int_{t_0}^{t_1} \dot{m}_{p,out}(t) r_k(t) dt \tag{3.36}$$

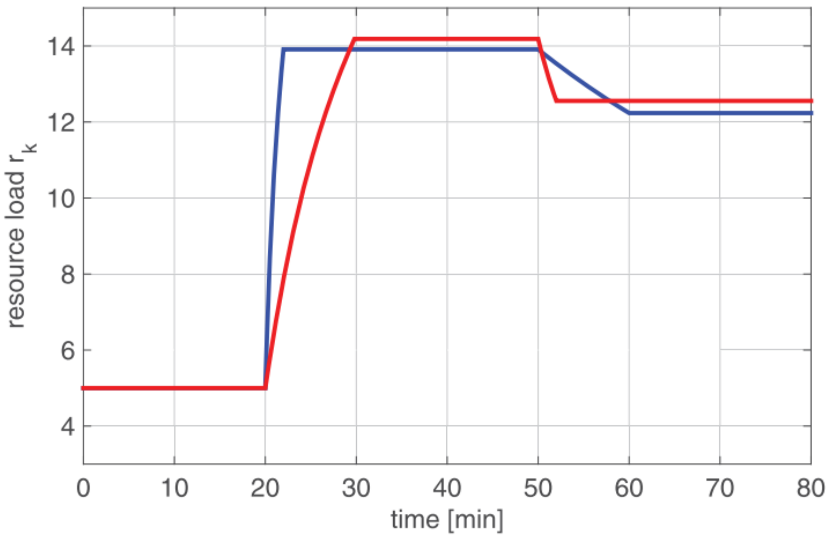

Figure 3.12: Resource load r_k per product m_p in the buffer tank for different transfer times (blue: $2min/10min$, red: $10min/2min$) for the same two batches with different efficiencies.

3.5 Application case: sugar plant

This section has been published as a case study in Kalliski and Engell (2017)[9]. The model was adapted from a previous work of Reinaldo Hernandez. The simulation study was performed by the intern Cristhian Oliveira under guidance of the author Marc Kalliski.

In the production of food-grade sugar from sugar beets, the beets are first shredded to increase the surface area for the subsequent extraction with hot water. Afterwards, the "fresh juice" is concentrated to "thick juice" by a multi-effect evaporator. In the next process step, the thick juice is further reduced in crystallizers until sugar crystals are formed. These are then separated from the molasses by a centrifuge and dried. Due to the high evaporation enthalpy of water, the process is energy-intensive and should therefore be made as efficient as possible by optimizing the energy and material efficiency. The model for the sugar plant is taken from a benchmark problem that was published by Mazaeda et al. (2014). It includes the evaporator-, crystallizer-, and a recovery-section (see Figure 3.13). The given plant is a hybrid production facility which is partly operated in batch and partly in continuous mode. In addition, there are two recycling streams that feed parts of the centrifuged molasses back into the process, thus improving material efficiency. These features complicate a resource efficiency analysis, as it is difficult to exactly determine the interrelationships at the boundary between the different operating modes. Moreover, the delay effects caused by the recycling streams have to be considered. Therefore, this application is suited to validate the method developed in chapter 3.4 for hybrid processes with recirculation.

3.5.1 Problem definition

In the first section the fresh juice passes through a cascade of three evaporators and is concentrated by the removal of excess water. The first stage is heated by an external steam supply and evaporates part of the water that is contained in the juice. By this step, steam is generated that can either be used to heat the next effect or to heat any of the crystallizers. Steam that is not used will be vented and its energy content is lost to the environment. The energy integration from effect to effect is possible, because of the increasing vacuum from effect to effect, making the separation less and less energy demanding. The sugar concentration in the rich juice is measured and controlled indirectly by the condenser pressure.

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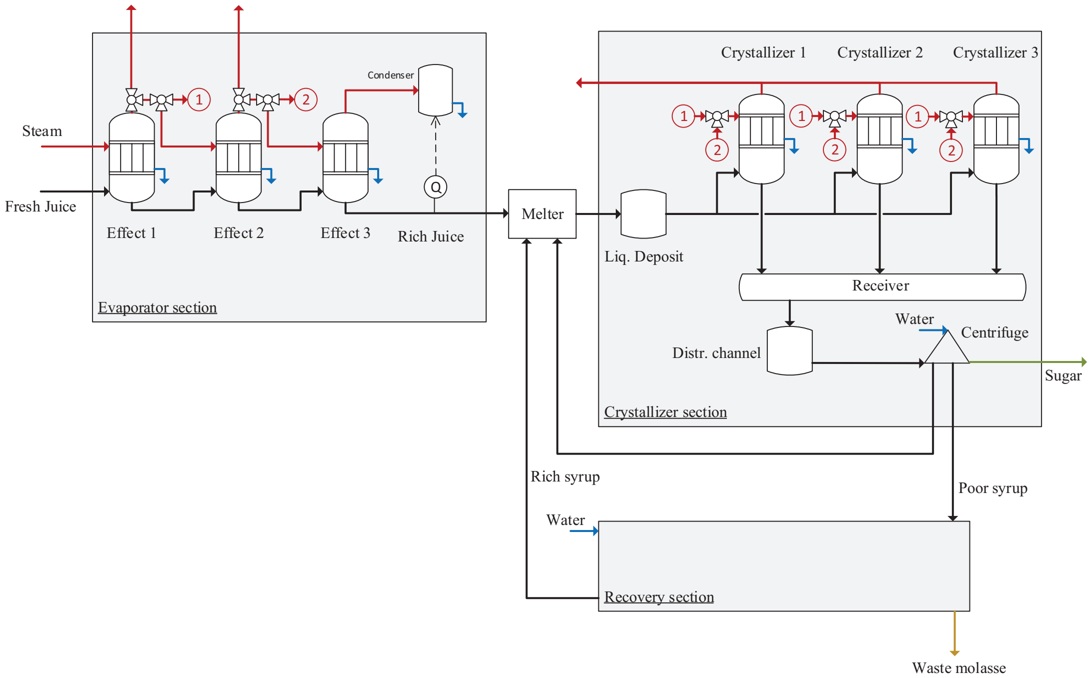

Figure 3.13: Flowsheet of the sugar plant for the production of food-grade sugar from sugar beets.

Subsequently, the concentrated juice is transferred to the melter, where it is blended with recycle streams that are also rich in sugar content. The melter is a continuously stirred vessel that blends the materials to feed them into the crystallizer section. After the liquid deposit, which is acting as a buffer tank, the syrup is charged into the discontinuously operated crystallizers which are operated in an alternating fashion. During the course of the batch-crystallization, more water is evaporated to obtain a supersaturated mixture and to initiate crystal growth. The heating energy for this task is supplied either by the first or by the second effect of the evaporator section. The suspended crystals from all units are collected in the receiver after the end of each batch. From there the mixture is continuously fed into the centrifuge via another buffer tank. The centrifuge is continuously operated and produces the product stream of sugar crystals and two additional syrup streams. The higher concentrated syrup is directly recycled to the melter, while the poor syrup is transferred to the recovery section. In a sugar plant, the recovery section usually consists of two sequential crystallizer sections that are identical in construction to the previously described crystallizer section. For the sake of simplicity these two stages are approximated by a continuous black-box model in the analysis of the benchmark problem.

3.5.2 Approach to resource efficiency

The system for the investigated application case comprises the complete plant with three subsections: the evaporator section, the crystallization section, and the recovery section. Water and sugar juice are the only raw materials that are used in the production of food-grade sugar (product). The waste stream (molasses) contains water, sugar, and impurities originating from sugar beets and is nontoxic, with little environmental impact. The indicators describing the resource efficiency of the process units are defined in Equations 3.37–3.43:

$$HEE_{evaporator} = \frac{\dot{m}_{sugar}}{\dot{Q}_{H,steam} - \left(\sum_i \dot{Q}_{generated,1,i} + \dot{Q}_{generated,2,i}\right)} \quad \forall i = 1,2,3 \tag{3.37}$$

$$HEE_{crystallizer,i} = \frac{\dot{m}_{sugar}}{\dot{Q}_{generated,1,i} + \dot{Q}_{generated,2,i}} \quad \forall i = 1,2,3 \tag{3.38}$$

Energy is introduced into the process at the evaporator section as steam $\dot{Q}_{H,steam}$. During the evaporation process, part of the sugar juice is evaporated and used to heat the crystallizers ($\dot{Q}_{generated,1}$ and $\dot{Q}_{generated,2}$). Thus, to calculate the evaporators heating efficiency ($HEE_{evaporator}$) $\dot{Q}_{generated,1}$ and $\dot{Q}_{generated,2}$ have to be deducted and accounted for in the calculation of the crystallizers heating efficiency $HEE_{crystallizer,i}$.

$$CEE_{evaporator} = \frac{\dot{m}_{sugar}}{\dot{Q}_{cool,condenser}} \tag{3.39}$$

Contributions to the cooling energy efficiency are considered at the condenser of the evaporator section ($CEE_{evaporator}$) and at each of the crystallizers ($CEE_{crystallizer,i}$) to condense the steam produced during the crystallization process:

$$CEE_{crystallizer,i} = \frac{m_{sugar}}{Q_{cool,condenser,i}} \quad \forall i = 1,2,3 \tag{3.40}$$

The material intensity relates the sugar in the juice that is fed to the process to the amount of solid sugar crystals that are exported from the crystallizer section:

$$MI_{sugar} = \frac{\dot{m}_{in,sugar}}{\dot{m}_{product,sugar}} \tag{3.41}$$

The water usage indicator captures the amount of water used by the process in the centrifuge of the crystallizer section and in the recovery section:

$$WU = \frac{\dot{m}_{water,in}}{\dot{m}_{sugar}} \tag{3.42}$$

$$WP_{molasse} = \frac{\dot{m}_{waste,molasse}}{\dot{m}_{sugar}} \tag{3.43}$$

The waste production is determined by the amount of molasses emitted by the recovery section which is necessary to discharge the impurities introduced to the system with the raw material. Because of the availability of a full dynamic model of the process, it is possible to calculate the exact resource efficiency of the (intermediate) product at any stage of the process by balancing and propagating pseudo-components as described in section 3 on the propagation of REIs between continuous and batch production. This approach has the advantage that closing the recycle streams does not pose any difficulties, because information on the resource consumption is available for all streams that enter the melter. If the amount of resources consumed per unit of the stream is below the current state of the pseudo-component in the melter, then the stream is reducing the value of the pseudo-state in the melter. This process is analogous to a stream of water diluting a reaction medium. For industrial applications, where such models may not be available, the contributions must be measured and subjected to data treatment to remove storage effects from the data. The environmental indicators are only of minor interest for the overall resource efficiency in this case, since the waste stream does not have a large environmental impact. Thus, the most important aspects for this process are the material and energy efficiency. The CEE and HEE are coupled in this setup and can be aggregated to the TEE without a loss of information, i.e. a minimized HEE will also yield a minimal CEE, because all the required cooling capacity in this process is directly proportional to the amount of heating applied. In order to obtain the resource optimal operation, the process was optimized for the total energy efficiency (TEE, eq. 3.44) and the material efficiency (MI_{sugar}, eq. 3.45) and compared to the base-case operation from the benchmark description. Here the variables $r_i(t)$ denote the resource intensities that are calculated from the resource utilization per product throughout the process (the inverse of the REI):

$$\begin{aligned} min_{B,P_i,p_{steam}} \frac{1}{TEE} = \\ min_{B,P_i,p_{steam}} \frac{\int_0^{t_{end}} r_{HEE}(t)\dot{m}_{product} + r_{CEE}(t)\dot{m}_{product} dt}{\int_0^{t_{end}} \dot{m}_{product} dt} \end{aligned} \tag{3.44}$$

$$\begin{aligned} min_{B,P_i,p_{steam}} MI_{sugar} = \\ min_{B,P_i,p_{steam}} \frac{\int_0^{t_{end}} MI_{sugar}(t)\dot{m}_{product} dt}{\int_0^{t_{end}} \dot{m}_{product} dt} \end{aligned} \tag{3.45}$$

3.5.3 Results

The decision variables for the operation of the process are shown in tab. 3.1, also indicating their limits and their base-case values. B is the brix set-point for the stream of juice after the evaporation section. The brix value is the mass-based concentration of the amount of solid material that is dissolved in water; here it includes sugar and impurities. The P-factors determine the actual pressures in the crystallizers during the execution of the recipes. These factors are multiplied with a pressure set-point trajectory in the crystallizers and increase or decrease the pressure. P-factors above 1 increase the pressure and thus the temperature within the crystallizers, resulting in shorter batch times. The brix and P-factor control inputs are parameterized by 12 piecewise-constant values each over the time horizon of $72,300s$ $(20h)$. The steam pressure of the imported steam can be varied between the bounds, but remains constant over the entire time horizon considered.

Table 3.1: Decision variables for optimization.

Symbol	Upper bound	Lower bound	Base-case	Parameterization	Type
B	72%	68%	70%	piecewise–const.	Continuous
P_1	1.2	0.8	1	piecewise–const.	Continuous
P_2	1.2	0.8	1	piecewise–const.	Continuous
P_3	1.2	0.8	1	piecewise–const.	Continuous
p_{steam}	$250kPa$	$180kPa$	$210kPa$	Time–invariant	Continuous

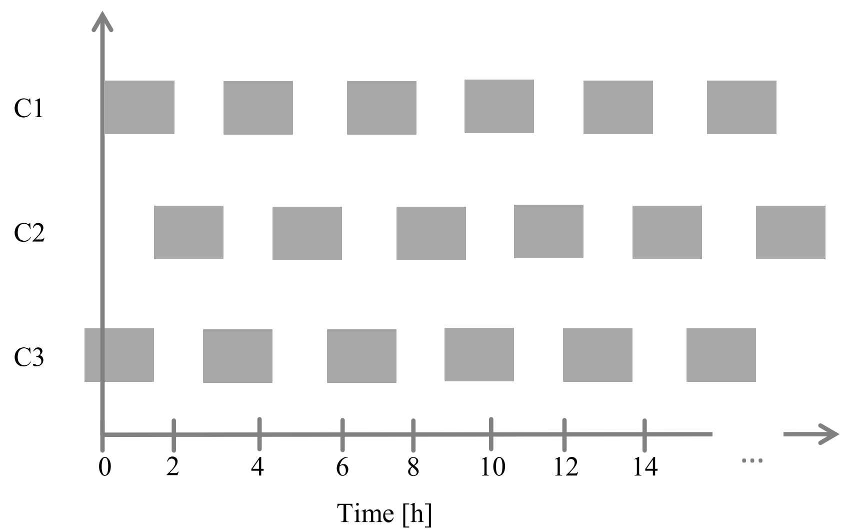

Figure 3.14: Crystallizer schedule.

The three crystallizers are started in an alternating fashion that is determined by a given schedule (see Figure 3.14). The length of the crystallization steps is varying according to the chosen P-factors. Due to the heat integration of the evaporation and crystallization sections, the pressure in the evaporators (and thus also the energy that is reused) is affected by the chosen P-factors. The model of the sugar plant includes the calculation of the resource efficiency. It is a DAE system with 151 differential and 1162 algebraic equations and is solved using the DASOLV solver for sparse DAE systems. The results of the optimization are summarized in table 3.2. The minimization of the total energy intensity improved the TEE by 1.2% and also slightly improved the MI in comparison to the base-case. The optimization for the MI of the raw material improved the indicator by 0.34% while also improving the environmental indicators. This was expected since an improved extraction of sugar from the raw material to the product reduces the sugar waste and reduces the water consumption for the recovery section. The overall improvements are small because of the tight constraints on the controlled variables and the relatively short optimization horizons starting after six discretization intervals. Nevertheless, the obtained information about the process can be exploited to supply a monitoring and decision support solution to the operators by displaying the current value in reference to the obtained optimum as defined in eq. 2.2. Figure 3.15 shows the optimal control inputs for the three cases.

Table 3.2: Optimization results for the objectives TEE and MI_{sugar}, compared to the base-case.

Objective	Values: $(TEE)^{-1}[kg/W]$	$MI_{sugar}[kg/kg]$	$WU[kg/kg]$	$WP[kg/kg]$
min $(TEE)^{-1}$	$\underline{4899.07}$	8954.37	4.324	4.681
min MI_{sugar}	5004.72	$\underline{8929.01}$	4.318	4.680
Base–case	4957.53	8959.78	4.323	4.680
Relative				
min $(TEE)^{-1}$	−1.18%	−0.06%	+0.02%	+0.02%
min MI_{sugar}	+0.95%	−0.34%	−0.12%	−0.11%
Base–case	100%	100%	100%	100%

During the first half of the optimization horizon the control inputs for the Brix- and P-values were forced to be equal to the base-case values to ensure numerical stability of the simulation runs during the optimization process. The fresh steam pressure is optimized for the entire horizon and assumes the values of 210 kPa (2.1 bar) (base-case), 250 kPa (2.5 bar) (TEE), and 180 kPa (1.8 bar) (MI) respectively. For the optimization of the total energy efficiency (TEE), the Brix value is maximized after the evaporator section. Overall, it seems to be more energy efficient to further concentrate the beet juice in the evaporators in order to start with a thicker solution in the crystallizers. With optimized material input (MI), on the other hand, the Brix value is minimized, resulting in lower losses of sugar via the purge stream of the recovery section. The optimization of the P-factors for the three crystallizers is less transparent. Mainly, they are determined by the timing offset of the crystallizer scheduling and the total amount of steam available from the evaporator section for heating the crystallizers. To further analyze the results of the optimization, it is necessary to extend the optimization horizon substantially to check whether the pattern of the selected P-factors is repeated and what average values are obtained per crystallization cycle.

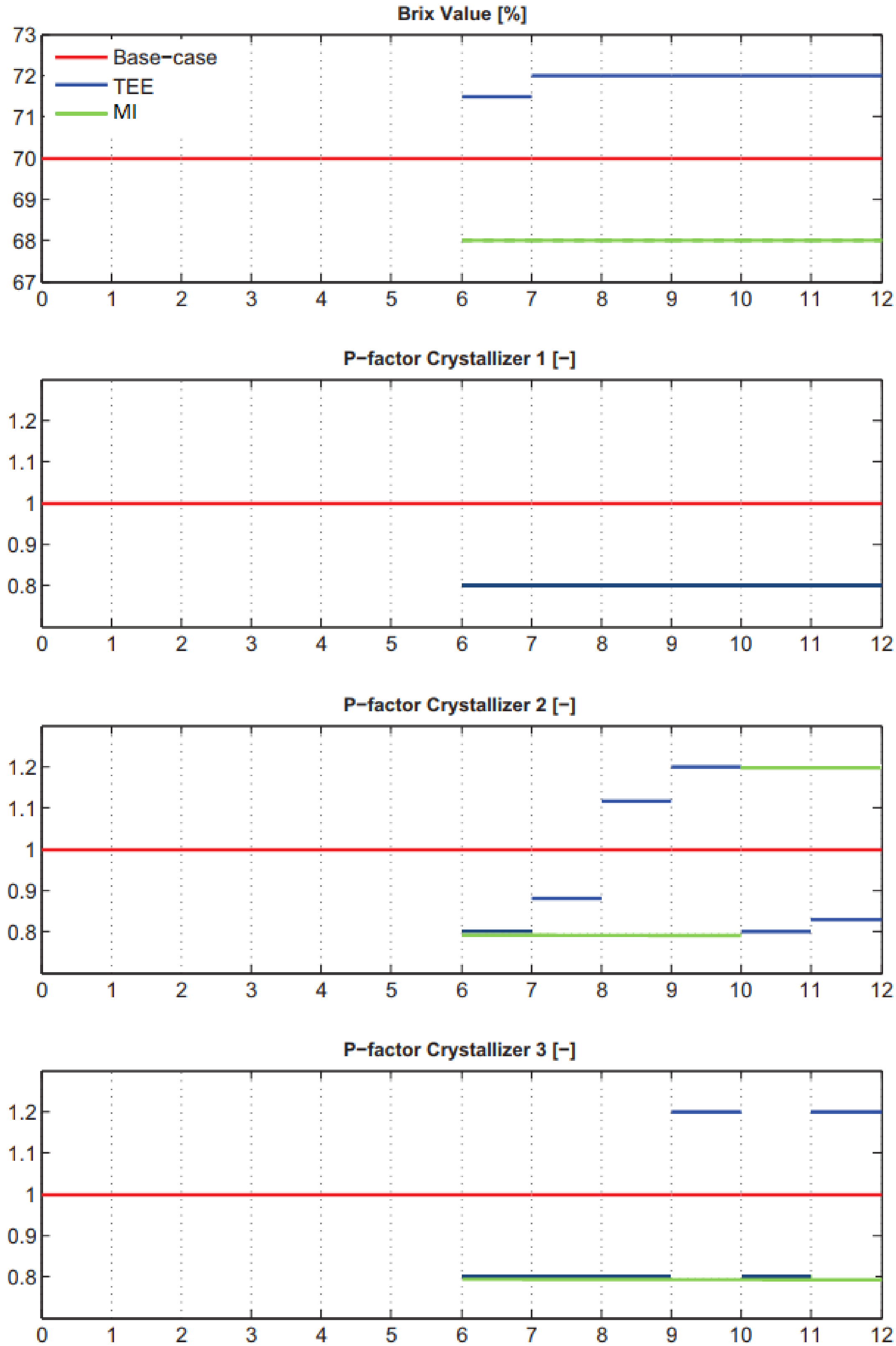

Figure 3.15: Optimized degrees of freedom for the sugar plant for different optimality criteria (optimization only performed for the second half of the time horizon).

3.5.4 Dashboard concept

In addition to the offline optimization of the production plant, the defined indicators and calculation rules can be used to display the current efficiency as well as its historical development. If this information is displayed to the operators in near real time in the form of a dashboard, it is possible to encourage them to react to inefficient operating conditions in the sense of decision support. For this purpose, a dashboard concept was developed for the sugar plant application case. Figure 3.16 shows the concept including a control panel for the navigation through the plant hierarchy with efficiency indicator bars for the three plant sections indicating the resource efficiency of each section (upper-left). Upon user interaction, the different plant sections can be activated, which triggers an update in the historical trends (lower-left) and the detailed view (upper- right) for the selected sub-section- and resource-specific REIs. The lower-right field is intended to give supplementary information about the visualization elements to increase the user acceptance. For the example shown in fig. 3.16, the user can identify a suboptimal performance of the crystallizer pans A1 and A2 in the crystallizer section. More detailed considerations regarding the development of efficient and effective decision support interfaces are outlined in chapter 5.

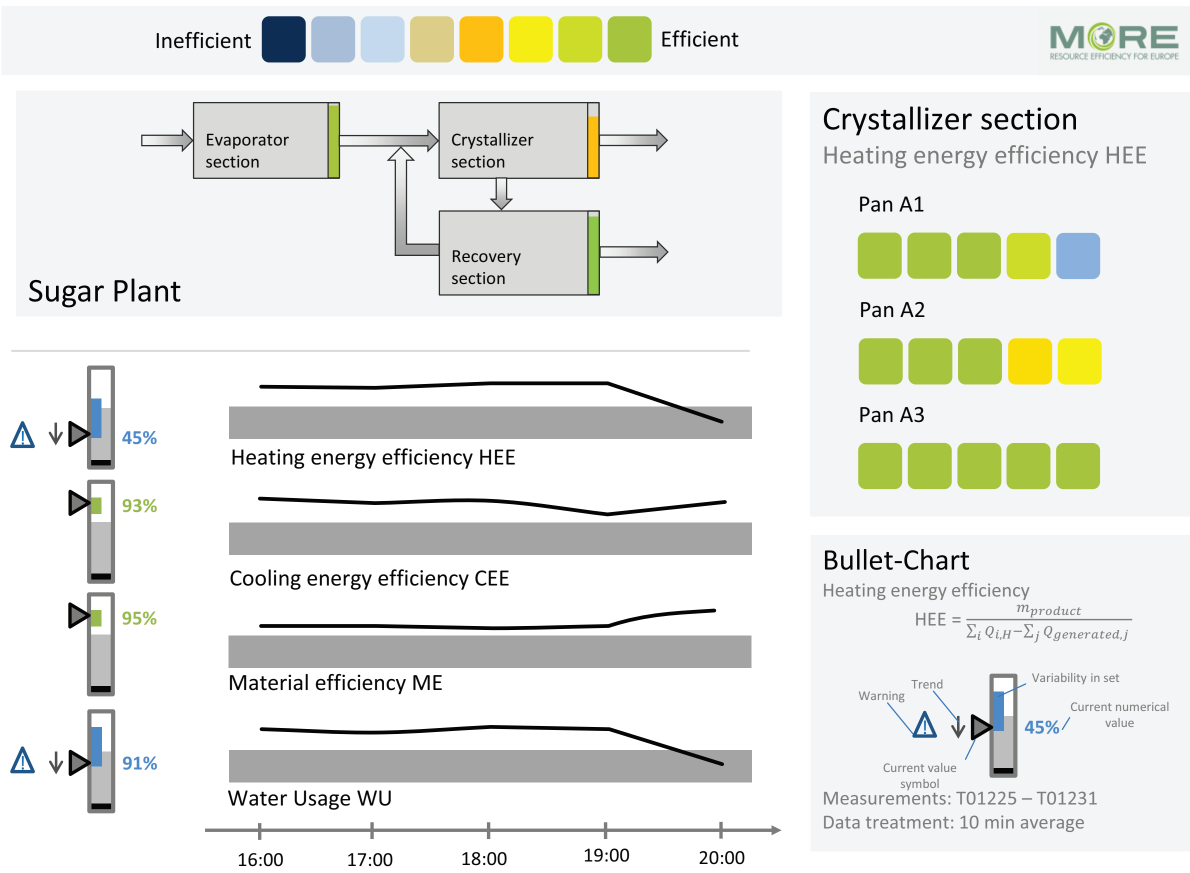

Figure 3.16: Dashboard concept for the sugar plant.

3.6 Conclusions

Parts of the conclusions were published in Kalliski and Engell (2017)[10].

In this chapter, a framework for the monitoring and optimization of resource efficiency in batch and mixed batch-continuous processing plants was developed. The streams of material and energy across the system boundary are the basis for the calculation of resource efficiency indicators (REIs), which reflect the technical performance regarding the transformation of energy and raw materials to products. Furthermore, they are complemented by environmental indicators that assess the waste production and emissions to air and water. The method proposes to evaluate the efficiency on unit level and aggregate or propagate the indicators to calculate the system-wide performance measures. When aggregated, the average unit performances are used to calculate the plant performance. Here, the chosen temporal resolution is uniformly used across the entire system, e.g. days. In comparison, this approach lacks accuracy for batch production facilities, since alternative production routes and optional recipe steps are not structurally represented and tracked. The preferred approach is indicator propagation that evaluates the process performance per unit and batch. By tracking the material throughout the plant and propagating the associated resource consumption it is possible to determine the performance of final product batches with respect to the considered REIs. All contributions that cannot be directly attributed to a specific batch are tracked by ORE indicators and will be uniformly distributed over the appropriate set of batches. The propagation approach requires a higher degree of effort in data acquisition, but allows to map and compare alternative process routes. Thus, real-time batch REIs can be used, locally, to optimize the efficiency of unit operations and the propagation results can be used to confirm that the local optimization efforts also improve the plant-wide performance. If a predictive plant model is available, global optimization schemes can be used to find the operational optimum.

Table 3.3 summarizes generic indicators the are applicable to most processing plants and classifies them into three levels: REIs on the batch level reflect the influence of the operational policies, such as the choice of set-points, trajectories, feeding policies, and timing of the transitions to the next unit operation. REIs on the batch-phase level characterize the performance of key production steps and can be used to investigate the root-cause of resource efficiency degradation or to identify the potential for improvements in crucial production steps. REIs on the plant level monitor contributions to the resource efficiency that results from production cleaning, scheduling, logistics or other plant-wide factors.

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Table 3.3: Overview of REI defined for batch processes.

Indicator	Abbreviation	Formula	Hierarchy level	Category
Overall resource efficiency	ORE_i	Case-specific	Plant level	Case-specific
Total material efficiency	TME	$\frac{m_{product}}{\sum_k m_{in,k}}$	Batch level	Material
Material input intensity	MI_k	$\frac{m_{in,k}}{m_{product}}$	Batch level	Material
Material efficiency	ME_k	$\frac{\sum_p m_{k,stoic,p}}{m_{in,k}}$	Batch level	Material
Material efficiency with recycle	$ME_{recycle,k}$	$\frac{\sum_p m_{k,stoic,p}}{m_{in,k}+(m_{in,recycle,k}-m_{out,recycle,k})}$	Batch level	Material
Total energy efficiency	TEE	$\left(\frac{1}{CEE}+\frac{1}{Hee}+\frac{1}{EEE}\right)^{-1}$	Batch level	Energy
Heat product	HP	$\frac{\sum_p Q_{generated,j}}{m_{product}}$	Batch level	Energy
Electrical energy efficiency	EEE	$\frac{m_{product}}{\sum_i W_{el,i}-\sum_j W_{generated,j}}$	Batch level	Energy
Cooling energy efficiency	CEE	$\frac{m_{product}}{\sum_m W_{cool,m}}$	Batch level	Energy
Heating energy efficiency	HEE	$\frac{m_{product}}{\sum_i Q_{H,i}-\sum_j Q_{generated,j}}$	Batch level	Energy
Total waste production	TWP	$\frac{\sum_j m_{waste,j}}{m_{product}}$	Batch level	Environmental
Water usage	WU	$\frac{m_{water,in}}{m_{product}}$	Batch level	Environmental
Waste production	WP_j	$\frac{m_{waste,j}}{m_{product}}$	Batch level	Environmental
Total reaction efficiency	TRE	$\sum_k \frac{\sum_p m_{k,stoic,p}}{m_{feed,k}}$	Phase level	Reaction
Reaction efficiency	RE_k	$\frac{\sum_p m_{k,stoic,p}}{m_{feed,k}}$	Phase level	Reaction
Purification energy efficiency	PEE	$\frac{m_{resid,S}+m_{resid,W}}{m_{feed,C}+m_{max,resid,W}}$	Phase level	Energy
		s.t. $m_{resid,W} \leq m_{max,resid,W}$		
Separation yield	SY_{CW}	$\frac{m_{product}}{Q_H+Q_{el}+W_{cool}}$	Phase level	Material

The presented real-time resource efficiency indicator framework can be used to derive REI that describe the efficiency of the entire process. In case a process model is available the indicators can be used as objectives to obtain the optimal operation regime of a plant with respect to each indicator. This was demonstrated on the industrial application case of a sugar plant in section 3.5. All inputs of materials and energy are considered and related to the amounts of products and intermediate products. The indicators are then propagated through the plant for individual batches and continuously operated sections to a plant-wide assessment. The propagation of indicators to plant-wide REIs reduces the number of indicators that describe the resource efficiency. For example, impacts of the chosen operating mode for the multi-stage evaporator are propagated along with the material to the crystallizer section. Here, additional effects from the re-circulation are considered alongside with the chosen operating mode in the crystallizers to achieve four efficiency indicators for the final product: (1) total energy efficiency TEE, (2) the material input intensity MI, (3) the water utilization WU, and (4) the waste production WP. The resource efficiency optimization conducted in this Chapter was performed individually for the two most important indicators TEE and MI by variation of the operational degrees of freedom listed in tab. 3.1. In both cases improvement potentials were identified with -0.34% for MI and -1.18% for TEE. From the economic point of view, the solution obtained for the optimization of TEE is preferable, because here both efficiencies improved and will have a positive impact on the economics. Of course this holds only true if the slightly reduced performance of WU and WP do not negate the savings. In order to find the true economic optimum the cost function could be altered to optimize the operating cost directly. Furthermore, a visualization concept was developed for how to present the resource efficiency indicators to operators and plant managers in an effective and efficient manner. This is especially important for batch processes because these processes are often not fully automatized and require continuous decision making by the operators. If supplemented with economic data, a well informed decision towards an optimized operation is possible.

The results of this application case show that it is possible to globally optimize the resource efficiency in mixed batch-continuous production facilities with the propagation concept developed in this thesis. In order to further improve the decision support, it would be beneficial to extend the indicator set by an economic indicator and solve the multi-criteria optimization problem to obtain the Pareto frontier. With this, the implementation of a decision support system is possible that supports the management to select an operating point among the Pareto optimal solutions. Here, the cost function either consists of one REI or of a weighted combination of multiple indicators, if the weighting factors are known *a priori*. Otherwise, a multi-criterial optimization is used to obtain a Pareto-optimal set of operating points. The set of optimal operating points reflects the trade-offs between possibly competing efficiency objectives and is the basis for DSS solutions that take managerial considerations into account.

Chapter 4

Multi-objective optimization of batch productions

The initial version of the MATLAB model was implemented in a supervised Master's thesis by Taher Sabry Elsayed Gomaa Ebrahim and later adapted for this work by the author. A Bachelor thesis by Jens Ehlhardt provided preliminary results regarding the Interface design. Furthermore, Jens Ehlhardt implemented parts of the MATLAB® graphical user interface as part of his duties as a student assistant, while the conceptual work was done by the author.

The selection of a suitable operating point is a management decision, where strategic goals can be considered that go beyond short-term financial benefits. As outlined in section 1.1 the operating point should be selected among the set of Pareto-optimal points. Based on the desired operating point, guidance for the optimal process inputs can be derived. This thesis proposes to consider the resource efficiency of a process in conjunction with its economic performance. The holistic description and optimization of resource efficiency for industrial processes requires a good understanding of the interactions with external resources and environmental impacts that are generated. Chapter 3 concluded that a minimal set of REIs should be defined in conjunction with an economic indicator in order to cover:

- the energy efficiency,
- the material efficiency and
- the environmental impact.

In order to account for the need to operate the process in a profitable state one should also include an indicator that reflects

- the economic benefit of the process.

Thus, for most application cases there will be more than one indicator resulting in a multi-dimensional description of resource efficiency. Trade-offs between competing interests are well known for technical systems: In general it is necessary to increase the reflux and boil-up ratio of a distillation column to increase the product recovery. Here, an improved recovery results in a better material efficiency at the cost of a decrease in energy efficiency, due to higher heating and cooling duties. Additionally, the production cost is of great interest in industrial applications and needs to be included in any consideration that aims to change the production process. Thus, the optimization of resource efficiency constitutes a multi-objective optimization problem. In general, processing plants can be operated at different operating points that are characterized e.g. by the choice of reaction conditions or the production scheduling. The variation of operating conditions does have an impact on the product formation, the economic performance, and the resource efficiency. The resulting solution space is the collection of all possible operation points with their corresponding REI values. The desired operational regime is the Pareto surface of this multi-dimensional space that describes the trade-off between competing targets, e.g. between the energy efficiency and the environmental performance if an off-gas treatment is energy intensive. An operating point is Pareto-optimal if any of the objectives (here REI) can only be improved at the expense of worsening another objective (Pareto, 1896, 2014).

This chapter uses an application case to elucidate the process of obtaining the Pareto frontier. It is based on the theoretical Williams–Otto process, initially proposed by Williams and Otto (1960) and later adapted by Forbes (1994) and Ebrahim (2015); Ebrahim et al. (2016) as a semi–batch reactor. This example is often used for benchmarking of control structures and optimization approaches, because of a relatively simple reaction system that still exhibits interesting dynamic behavior and potential for optimization. First, the Williams–Otto process is introduced in section 4.2.1, including the interpretation regarding resource efficiency. Subsequently, the model is used for the derivation of indicators (section 4.2.2), and the Pareto optimization (section 4.2.3). The results will be the basis for the development of a suitable human machine interface in Chapter 5.

4.1 State-of-the art

As indicated in section 1.1 the optimization of resource efficiency is by definition a multi-dimensional entity with possibly competing interests that need to be negotiated. The optimization problem can either be addressed by mapping the multi-dimensional objective function to a single objective function or by obtaining the full set of Pareto-optimal solutions. Since, the individual preferences regarding the weighting between the different objectives are a constantly reevaluated managerial decision, decision support systems for the multi-dimensional case should address the full problem and supply the Pareto optimal set of solutions. The basic concepts are discussed in section 4.1.1 and an approach to obtain the Pareto frontier in 4.1.3.

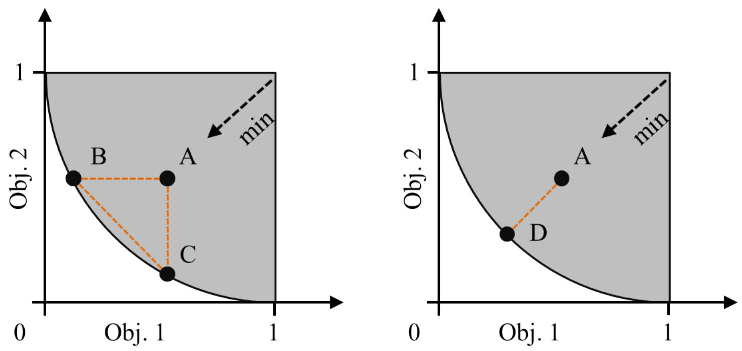
The goal of multi-criteria optimization is to obtain the Pareto front where a compromise between competing interests of the objective functions has to be found. Based on this, decision support can then be generated that helps the user to act Pareto-optimal on the one hand, and to make an informed choice of an operating point on the other hand. Section 4.1.1 discusses approaches from the literature to solve multi-objective optimization problems in order to achieve the most uniform coverage of the Pareto front. Regardless of the approach, the resulting optimization problems must be solved, which consist of the dynamic optimization of a batch process. Therefore, Section 4.1.2 introduces the concept of control vector parametrization (CVP), which can be used to reduce the number of manipulated variables and results in a non-linear program (NLP). Section 4.1.3 presents the normalized-normal-constraint (NNC) method, which is used in section 4.2 to solve an application case.

4.1.1 Multi-criteria optimization

Messac et al. (2003) distinguish two classes of approaches to solve multi-criteria optimization problems. The first class uses an objective function that takes all competing interests into account. If properly formulated the objective function contains all preferences of the designer. Often this is done in an iterative fashion, by adjusting numerical weights until the user is satisfied with the result obtained and the design process ends with an optimal solution (Osyczka and Kundu, 1995; Cheng and Li, 1998; Srinivasan and Tettamanzi, 1996; Messac, 1996). A common approach to balance the influences is economic optimization that considers all interests by the associated cost (Idris and Engell, 2012). For economic optimization problems a global optimum does exist, additional local optima may coexist. This approach is useful to obtain a cost efficient design for chemical production plants.

The second class of approaches aims to find a set of optimal solutions for all possible weight combinations. Subsequently, a solution can be selected among the set of optimal points. The balancing of resource efficiency aspects is a reoccurring managerial decision making process, where the priorities (weights) may be under constant reevaluation. Thus, the set of optimal solutions can be revisited if priorities regarding resource efficiency shift. In other words, the goal of the second class of approaches is to obtain a set of solutions that describes the boundary of the feasible region towards improved objectives. On the boundary towards improved performance, trade-offs between competing interests (objectives) are active, where an improvement of one must result in the deterioration of at least one other objective. Solutions that possess this property are called Pareto optimal, while the set of solutions is referred to as Pareto frontier (Pareto, 1896, 2014). Figs. 4.1a–

4.1b show the feasible region for a two-dimensional minimization problem. The border of the feasible region toward the origin is the Pareto frontier. This translates to a multi-objective optimization problem, with different aspects of resource efficiency as objectives. It is generally desirable to operate the process on the Pareto frontier since a suboptimal operating point A can be improved on each objective without deteriorating another (see points B, C and D in figs. 4.1a–4.1b). Comparing Pareto optimal solutions B and C in fig. 4.1a, the principal of Pareto optimality becomes obvious: starting at B objective 2 can only be improved (reduced), while deteriorating objective 1 (point C).



(a) Example 1. (b) Example 2.

Figure 4.1: Two-dimensional Pareto frontier for a minimization problem. The gray area depicts the feasible region. The border towards the origin is the Pareto frontier.

Messac et al. (2003) summarizes different methods to obtain the solutions on the Pareto frontier:

- Weighted sum (WS) method
- Normal boundary intersection (NBI) (Das and Dennis, 1997)
- Physical programming (PP) (Messac, 1996; Messac and Mattson, 2002)
- Compromise programming (CP) (Chen et al., 1999)
- Genetic algorithms (GA) (Osyczka and Kundu, 1995; Eskandari and Geiger, 2007)
- Normal constraint (NC) method (Messac et al., 2003)
- Normalized normal constraint (NNC) method (Messac et al., 2003; Messac and Mattson, 2004)

The WS method is the simplest approach. It defines an aggregated cost function and varies the corresponding weights to track the Pareto frontier. While being easily applicable to a broad variety of problem formulations and solvers, it fails for non-convex Pareto frontiers, because it tends to find only extreme points of the front with better values for the overall cost function. Thus, the approach is not suitable to obtain good coverage. The form of the Pareto front is not known *a priori* and thus we cannot assume convexity for resource efficiency optimization problems and must use a method that is robust against non-convex problems. Furthermore, even for convex problems a uniform distribution of solutions on the front is not guaranteed, because it is sensitive to the objectives' scaling.

GA approaches, combined with Pareto filtering, can be used to generate Pareto frontiers. However, GA approaches require tuning and a lot of computational time to ensure an even distribution and confidence that the current set of solutions is sufficiently close to the true Pareto front. According to Messac et al. (2003) *"[...] the NBI method is more prone to generating dominated solutions than is the NC method [,...]"*, while *"the development of the PP algorithm is not trivial"* for most application cases.

CP and the NC method have shown to be suitable for non-convex-cases but lack a good distribution of solutions, if the sensitivities close to the individual optima are significantly different (Messac and Ismail-Yahaya, 2001). The NNC method overcomes this shortcoming by normalizing the design space (Messac et al., 2003). Furthermore, the NNC is only introducing additional constraints, without any interference with the algorithm that is used to solve the optimization problem. The NNC method is highly practical and is summarized in subsection 4.1.3.

4.1.2 Control vector parametrization

Control Vector Parameterization (CVP) is used to convert optimal control problems to nonlinear programs (NLP) by discretizing the control inputs (Ray, 1989). The control inputs profile is optimized with respect to the process constraints and is evaluated according to an objective function. In optimal control problems, the system behavior is described by a set of ordinary differential equations that are numerically integrated. According to Ray (1989) the parametrization is usually conducted based on piece-wise constant or polynomial expressions. Eq. 4.1 shows a B-spline formulation for the input discretization (Boor, 2001).

$$u_i(t) = \sum_{j=1}^{n_i} u_{i,j}\phi_j^m(t) \tag{4.1a}$$

$$\phi_j^m(t) = \frac{t-\tau_j}{\tau_{j+m-1}}\phi_j^{m-1}(t) + \frac{\tau_{j+m}-t}{\tau_{j+m}-\tau_{j+1}}\phi_{j+1}^{m-1}(t) \tag{4.1b}$$

$$\phi_j^1(t) = \begin{cases} 1 & \text{if} \quad \tau_j \leq t < \tau_{j+1} \\ 0 & \text{otherwise} \end{cases} \tag{4.1c}$$

According to eq. 4.1a the inputs $u_i(t)$ are expressed as a linear combination of the product $u_{i,j}\phi_j^m(t)$ for all inputs i, where $u_{i,j}$ is the decision variable in the optimization problem and $\phi_j^m(t)$ B-splines of order m. The index j is running over the n_i discretization intervals. The definition of $\phi_j^m(t)$ in eq. 4.1b includes spines of the reduced order $m-1$

and additional discretization intervals τ_{j+m-1} and τ_{j+m}. Thus, higher orders of B-splines considered in eq. 4.1a will result in a smoother representation of the input profile. In case of piece-wise constant input parametrization (see eq. 4.1c), the order is $m = 1$ and the decision variable $u_{i,j}$ are equal to the control input u_i during the corresponding time interval j: $\tau_j \leq t < \tau_{j+1}$. Additional constraints are need to ensure compliance with the process constraints on and between the discretization points (Schlegel et al., 2005).

In the scope of the application case in section 4.2.3 a piece-wise constant approach was used with the numerical integrator ode45 (Dormand and Prince, 1980; Shampine and Reichelt, 1997). The optimization was performed using the TOMLAB optimization toolbox for MATLAB® with the solver SNOPT. SNOPT depends on a sequential quadratic program (SQP) that is suitable for large scale problems. The gradients are obtained by finite differences if not supplied by the user (Gill et al., 2015).

4.1.3 Normalized-normal-constraint method

Decision support concerning multi-objective optimization problems requires the generation of Pareto optimal operating points with respect to the objectives, here the REIs. The goal is to obtain evenly distributed points on the Pareto frontier (see subsection 4.1.1). In this thesis the normalized normal constraint (NNC) method is used to achieve this goal (Messac et al., 2003). It is advantageous over other MO optimization algorithms, because it is capable to generate evenly distributed Pareto-optimal points for convex and non-convex optimization points with little effort.

$$\min_{x} \quad \mu_i(x) \tag{4.2a}$$

$$s.t. \quad g_j(x) \leq 0 \tag{4.2b}$$

$$h_k(x) = 0 \tag{4.2c}$$

$$x_{li} \leq x_i \leq x_{ui} \tag{4.2d}$$

The normalized normal constraint method is a two stage approach to an n-dimensional MO optimization. The idea in the first stage is to introduce $n-1$ additional constraints that are orthogonal to an n-dimensional hyperplane that is defined by the individual optima of the optimization problems PU_i, called anchor points μ^{i*} (see eq. 4.2). The $(n-1)$ inequality constraints intersect in the hyperplane points $\bar{X}_{pj}$ with $p \in 1, 2, ..., m_1$, where m_1 is a predefined number of desired Pareto-points. Fig. 4.2 shows the construction of the hyperplane for two objectives. For each Pareto-point an optimization problem is solved that considers one of the original objectives and the additional normalized normal constraints. The inequality constraints are formulated to constrain the feasible solution space towards the anchor point μ^{i*} that corresponds to objective i. Thus, evenly distributed hyperplane points will yield a comparably well distributed set of Pareto optimal solutions.

The algorithm for the generation of candidate solutions is summarized in tab. 4.1. For a graphical representations of the process, the reader is referred to the original contribution of Messac et al. (2003).

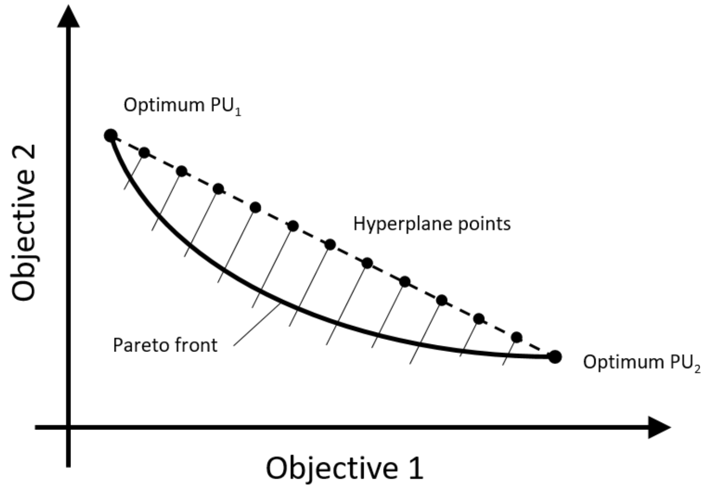


Figure 4.2: Two-dimensional representation of the NNC approach, for a minimization problem with two objectives.

$$\min_{x} \quad \bar{\mu}_n \tag{4.3a}$$

$$s.t. \quad g_j(x) \leq 0 \tag{4.3b}$$

$$h_k(x) = 0 \tag{4.3c}$$

$$x_{li} \leq x_i \leq x_{ui} \tag{4.3d}$$

$$\bar{N}_k \left(\bar{\mu} - \bar{X}_{pj}\right)^T \leq 0 \tag{4.3e}$$

$$\bar{\mu} = \{\bar{\mu}_1(x), ..., \bar{\mu}_n(x)\} \tag{4.3f}$$

In the second stage the obtained candidate solutions from the algorithm in tab. 4.1 are checked for Pareto-optimality. Using the notation introduced above, Messac et al. (2003) outlined global Pareto-optimality by:

> “A design metric vector μ^* is globally Pareto optimal if there does not exist another design metric vector μ such that $\mu_j \leq \mu_j^*$ for all $i \in \{1, 2, ..., n\}$, and $\mu_j < \mu_j^*$ for at least one index of $j, j \in \{1, 2, ..., n\}$ in the feasible design space.”

The filter algorithm iterates over all candidate solutions. If any of the other solutions dominate the current solution, it is discarded. A point is said to be dominant if at least one objective is better without another objective worsening. After the algorithm iterated trough all candidate solutions, the remaining points are in the set of Pareto optimal solutions.

Table 4.1: Normalized normal constraint method for n-objective case, according to Messac et al. (2003).

Algorithm step	Description
1 – Anchor points	The anchor points μ^{i*} are obtained by solving an individual optimization problems (see eqns. 4.2) for each objective $i \in 1, 2, ..., n$, where n is the number of objectives. The hyperplane defined by the anchor points is defined as utopia plane.
2 – Normalization	To avoid scaling deficiencies the optimization is performed on a normalized space. The scaling is performed with reference to the utopia (μ^u) and nadir points (μ^N), with: $\mu^u = [\mu_1(x^{1*}) \;\; \mu_2(x^{2*}) \;\; \cdots \;\; \mu_n(x^{n*})]^T$ $\mu^N = \begin{bmatrix}\mu_1^N & \mu_2^N & \cdots & \mu_n^N\end{bmatrix}^T$ where $\mu_i^N = max\,[\mu_i(x^{1*}), \mu_i(x^{2*}), \cdots, \mu_i(x^{n*})] \qquad \forall i \in \{1, 2, ..., n\}$ We obtain the scaled metrics $\bar{\mu}_i$: $\bar{\mu}_i = \frac{\mu_i - \mu_i(x^{i*})}{l_i} \qquad \forall i \in \{1, 2, ..., n\}$ with $L = [l_1, l_2, ..., l_n]^T = \mu^N - \mu^u$ Here, $x^{i*} \in \mathbb{R}$ denotes the optimal decision vector.
3 – Utopia plane vectors	The utopia plane vectors $\bar{N}_k$ define the directions from all $\bar{\mu}^{k*}$ to a selected $\bar{\mu}^{n*}$ for $k \in \{1, 2, ..., n-1\}$, by: $\bar{N}_k = \bar{\mu}^{n*} - \bar{\mu}^{k*}$.
4 – Normalized increments	The discretization increment δ_k along $\bar{N}_k$ is chosen in relation to the number of points m_1 along $\bar{N}_1$: $\delta_k = \frac{1}{m_k - 1}$, with $m_k = \frac{m_1 \lVert \bar{N}_k \rVert}{\lVert \bar{N}_1 \rVert}$.
5 – Hyperplane points	Evenly distributed hyperplane points are calculated by: $\bar{X}_{pj} = \sum_{k=1}^{n} \alpha_{kj} \bar{\mu}^{k*}$, where $0 \leq \alpha_{kj} \leq 1$, $\sum_{k=1}^{n} \alpha_{kj} = 1$.
6 – Pareto points	Each of the j Pareto solution candidates is obtained by solving the optimization problem defined in eqns. 4.3. If gradient based methods are used, the performance can be improved by smart initialization from Monte Carlo simulation or previously obtained Pareto solutions.
7 – Obtain objective values	The objective function values μ_i corresponding to the normalized candidates $\bar{\mu}_i$ are obtained according to: $\mu_i = \bar{\mu}_i l_i + \mu_i(x^{i*})$

4.2 Williams-Otto semi-batch reactor example

The Williams–Otto process was initially introduced as a continuously operated process example to test computer-based control strategies. It was designed to be simple enough for a fast and convenient implementation while also exhibiting interesting system dynamics (Williams and Otto, 1960). Würth et al. (2009), Ebrahim (2015) and Ebrahim et al. (2016) modified the original Williams–Otto reactor benchmark into the form of a semi-batch reactor to investigate control structures for batch processes. In this work, the Williams–Otto semi-batch reactor (WOSBR) serves as a use case to demonstrate the applicability of multi-objective optimization methods with respect to resource efficiency. Thus, the resource efficiency indicator framework developed in Chapter 3 is combined with state-of-the-art approaches to multi-objective optimization methods to find the best process parameters to maximize the resource efficiency indicators.

4.2.1 Problem definition

The reaction system consists of three exothermic and irreversible reactions (eqs. 4.4–4.6). In the first reaction the raw materials A and B are converted equimolarly to an intermediate C that in turn reacts with another mole of B to the products P and E. A competing side reaction depletes part of the product P under consumption of C to a waste product G. All three reactions have temperature dependent reaction rates according to the Arrhenius equation (eq. 4.8e). In order to introduce an environmental impact to the case, the waste product G is considered here to be toxic and hence should be avoided.

$$A + B \xrightarrow{k_1} C \tag{4.4}$$

$$C + B \xrightarrow{k_2} P + E \tag{4.5}$$

$$P + C \xrightarrow{k_3} G \tag{4.6}$$

In this thesis, the semi-batch operation mode is considered, where the raw material A is placed inside of the reactor prior to the reaction start. Later the raw material B is added to the mixture to start the reaction process. The reaction dynamics can be influenced by changing the feed profile as well as the heating and cooling profile of the reactor (cf. fig. 4.3). Since the reaction rates r_i are dependent on the reactor temperature T_R and the concentrations of the reagents, the control inputs also affect the final composition of the mixture and subsequently the resource efficiency.

The process dynamics are captured in the model equations 4.7a–4.7h. Here, V represents the current liquid volume, M_{tot} the total mass contained in the reactor, MW_i the molecular weight, and m_i the mass of the species i.

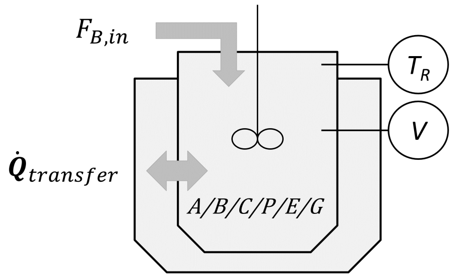


Figure 4.3: Schematic representation of the Williams–Otto semi-batch reactor with the inflowing mass of raw material B ($F_{B,in}$), heat transfer $\dot{Q}_{transfer}$, the reactor temperature T_R, the liquid content V, and species contained in the reactor.

$$\frac{dV}{dt} = \frac{F_{B,in}}{\rho} \tag{4.7a}$$

$$\frac{dm_A}{dt} = -r_1 M_{tot} \tag{4.7b}$$

$$\frac{dm_B}{dt} = -\frac{MW_B}{MW_A} r_1 M_{tot} - r_2 M_{tot} + F_{B,in} \tag{4.7c}$$

$$\frac{dm_C}{dt} = \frac{MW_C}{MW_A} r_1 M_{tot} - \frac{MW_C}{MW_B} r_2 M_{tot} - r_3 M_{tot} \tag{4.7d}$$

$$\frac{dm_E}{dt} = \frac{MW_E}{MW_B} r_2 M_{tot} \tag{4.7e}$$

$$\frac{dm_G}{dt} = \frac{MW_G}{MW_C} r_3 M_{tot} \tag{4.7f}$$

$$\frac{dm_P}{dt} = \frac{MW_P}{MW_B} r_2 M_{tot} - \frac{MW_P}{MW_C} r_3 M_{tot} \tag{4.7g}$$

$$\frac{dT_R}{dt} = \frac{H}{V C_P \rho} \tag{4.7h}$$

The reaction rates r_i in eq. 4.7b–4.7g are temperature dependent according to Arrhenius laws (eq. 4.8e) and a function of the mass fractions x_i of the reagents that are consumed in each specific reaction:

$$r_1 = k_1 x_A x_B \tag{4.8a}$$

$$r_2 = k_2 x_B x_C \tag{4.8b}$$

$$r_3 = k_3 x_C x_P \tag{4.8c}$$

$$x_A = \frac{m_A}{M_{tot}}, x_B = \frac{m_B}{M_{tot}}, x_C = \frac{m_C}{M_{tot}}, x_P = \frac{m_P}{M_{tot}} \tag{4.8d}$$

$$k_i = a_i exp\left(\frac{-b_i}{T_R + T_{ref}}\right), \qquad i = 1, 2, 3 \tag{4.8e}$$

$$M_{tot} = m_A + m_B + m_C + m_E + m_G + m_P \tag{4.8f}$$

The change in the reactor temperature is a result of the energy balance in eq. 4.7h. H is calculated according to eq. 4.9 as a function of the heat effect of the three reactions, the addition of raw material B and the transferred heat $Q_{transfer}$. The isobaric specific heat C_p is assumed to be constant. The Arrhenius parameters a_i, b_i, T_{ref} and all other relevant parameters are listed in tab. A.1 in the appendix.

$$\begin{aligned} H = F_{B,in} C_P \left(T_{in} - T_R\right) - \Delta H_1 r_1 M_{tot} - \Delta H_2 r_2 M_{tot} \\ - \Delta H_3 r_3 M_{tot} + Q_{transfer} \end{aligned} \tag{4.9}$$

Furthermore, the process is subject to the constraints shown in eqs. 4.10a–4.10e, including restrictions on the feed rate, the heating and cooling rates, the reactor temperature, and the maximal volume. A minimal product formation $m_P(t_f)$ at the end of the batch (time $t_f = 1500s$) is imposed to ensure a certain product quality.

$$0 \ \frac{kg}{s} \leq F_{B,in}(t) \ \leq 5.784 \ \frac{kg}{s} \tag{4.10a}$$

$$-600 \ kW \leq Q_{transfer}(t) \leq 800 \ kW \tag{4.10b}$$

$$20 \ ^\circ C \leq T_R(t) \quad \leq 90 \ ^\circ C \tag{4.10c}$$

$$V(t_f) \quad \leq 5 \ m^3 \tag{4.10d}$$

$$m_P(t_f) \quad \geq 50 \ kg \tag{4.10e}$$

4.2.2 Indicator development

The resource efficiency is dependent on the definition of the system boundary, its interaction with the environment, and the goal of the process as required by the principles in section 2.2.2. In the present case the balancing volume encompasses the liquid volume in the reactor (cf. fig. 4.4) for the duration of one batch each that is fixed at $t_f = 1500s$. Any possible heat losses around the reactor or material losses in the post processing of the resulting compound mixture are neglected for this example.

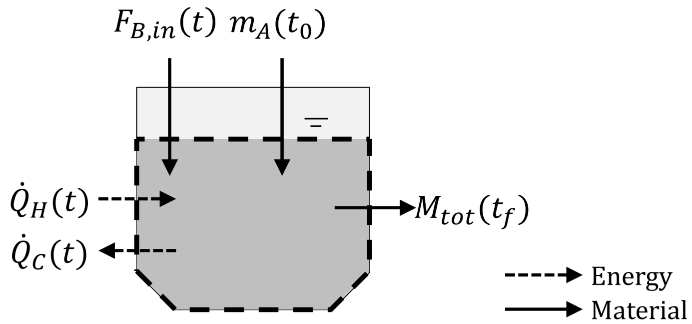


Figure 4.4: Balancing volume in the Williams–Otto semi-batch reactor.

Total material efficiency
The assessment of the material efficiency is based on the material balance of the process

or process step. Equation 3.1 generally defines REIs as the ratio of the generated product and the consumed amount of resources. Figure 4.4 shows that the mass balance for the Williams-Otto semi-batch reactor (WOSBR) is determined by the amount of product mixture $M_{tot}(t_f)$ at the end of the batch and the material streams of raw materials A and B. From the reaction equations 4.4–4.6 the species A and B are identified as reactants and thus classified as resources. For this application case, the valuable components P and E are considered as products of the process. Consequently, the "total material efficiency" (TME) is defined according to eq. 4.11, which is dependent on the pre-charged amount $m_A(t_0)$, the integral of the dosed amount of B $F_{B,in}$, and the final product amounts $m_P(t_f)$ and $m_E(t_f)$.

$$TME = \frac{m_{P,end} + m_{E,end}}{m_{A,tot} + m_{B,tot}} = \frac{m_P(t_f) + m_E(t_f)}{m_A(t_0) + \int_0^{t_f} F_{B,in}(t)dt} \tag{4.11}$$

As a consequence, the material efficiency improves for a higher product yield regardless if the amounts of P or E increase. Since both valuable products enter into the consideration, the indicator is termed "total material efficiency" (TME).

Total energy efficiency

The effects relevant for the energy efficiency are the obtained mass of products and the transferred energy, whereby the heating and cooling duty are not explicitly distinguished. In case of a technical application case it would be sensible to first convert both duties in primary energy according to their steam level or type of cooling agent and temperature level. For the WOSBR the "total energy efficiency" (TEE) is defined according to eq. 4.12, based on the energy needed to heat the pre-charged raw material A to the initial conditions as well as the integral over the heating and cooling duties $\dot{Q}_H$ and $\dot{Q}_C$ over the course of the batch. Again, the obtained amounts of P and E are used as product.

$$TEE = \frac{m_{P,end} + m_{E,end}}{Q_H + Q_C} = \frac{m_P(t_f) + m_E(t_f)}{Q_{H,init} + \int_0^{t_f} \dot{Q}_H(t) + \dot{Q}_C(t)dt} \tag{4.12}$$

Environmental performance

In the problem definition (cf. section 4.2.1) the component G is described as toxic and hence qualifies as an environmental impact if obtained through the reaction. The environmental performance indicator (ECO) is defined in eq. 4.13 to monitor its formation. Analogously to the preceding indicators, the product is captured by considering $m_P(t_f)$ and $m_E(t_f)$ and referenced against the amount of G in this case.

$$ECO = \frac{m_{P,end} + m_{E,end}}{m_{G,end}} = \frac{m_P(t_f) + m_E(t_f)}{m_G(t_f)} \tag{4.13}$$

The ECO indicator grows for an improved performance, which is a result of increased product formation or lower product specific formation of the side product G.

Benefit

Finally, the benefit (BEN) for the reaction process is specified to capture the economic performance that is the motivation behind the operation of all processes in the chemical industry. Positive contributions to the benefit are associated with the product revenue for P and E. The remaining amount of C is waste, but creates a small revenue as fuel, e.g. in a steam generation process. The raw material expenses, utility costs, and cost for the side product disposal of G are reducing the earnings. The remaining amount of A and B can be separated and disposed of at no cost.

$$\begin{aligned} BEN = & \left[-c_A,\ -c_B,\ c_C,\ c_E,\ -c_G,\ c_P,\ -c_{QC},\ -c_{QH}\right] \\ & \cdot \left[m_A(t_0),\ \int_0^{t_f} F_{B,in}(t)dt,\ m_C(t_f),\ m_E(t_f),\ m_G(t_f),\ \int_0^{t_f} \dot{Q}_C(t)dt,\ \int_0^{t_f} \dot{Q}_H(t)dt\right]^T \end{aligned} \tag{4.14}$$

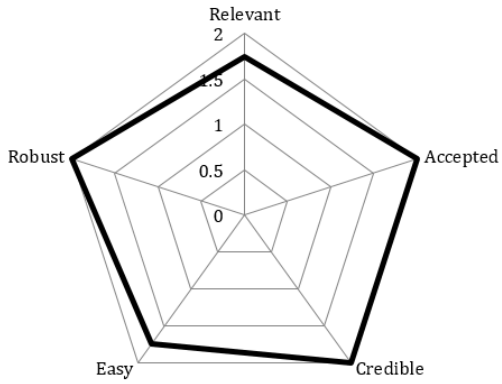
The prices used for the calculation of the benefit can be found in tab. A.2 of the appendix.

RACER Analysis

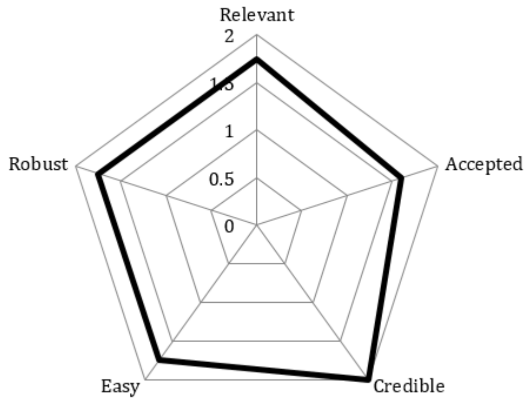
In accordance with the methodology outlined in section 2.2.3, the REIs are checked for the RACER criteria: Relevance, Acceptance, Credibility, Easiness, and Robustness to determine the suitability for online monitoring and control purposes. The analysis identifies weaknesses in the definition of the indicators that require attention or countermeasures during the indicator life cycle.

The RACER analysis was conducted by the author and the results are summarized in figs. 4.5a–4.5c for inspection. The indicators were assessed in all five categories with the standardized RACER survey and rated on a scale between zero (not achieved) and 2 (fully achieved). The detailed evaluation is documented in tab. B.1 and figs. B.1–B.18 in the appendix B.

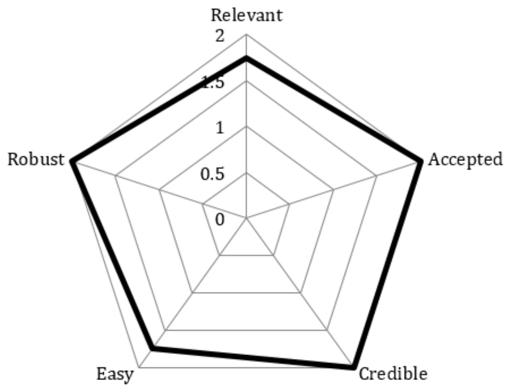
The TME and ECO indicators perform well in the analysis, there are only minor deductions in the categories relevance and easy. The relevance is reduced because it is not entirely transparent how the manipulated inputs are affecting the indicators. With respect to the category easy, points are reduced, since the concentration of product P and component G at the end of the reaction process is needed for the calculation of the indicators. This information is usually not readily available and must be obtained through expensive online measurements, delayed laboratory analysis or a mathematical model to estimate the reaction outcome based on the measured variables.



(a) Radar plot for TME.



(b) Radar plot for TEE.



(c) Radar plot for ECO.

Figure 4.5: RACER scores for the investigated REIs: total material efficiency (TME), total energy efficiency (TEE), and the eco-performance indicator (ECO). The numerical values are listed in tab. B.1 of the appendix B.

Regarding the energy efficiency additional points for acceptance are reduced. Technical personnel might argue against the simplification that the required amount of heating and cooling is simply lumped into the indicator. As discussed earlier a conversion to primary energy is an option, but was disregarded here due to the theoretical nature of this case. A similar reasoning leads to reductions for robustness, because the required heating and cooling duty are not considered separately. The decision to lump both contributions into one indicator was made to reduce the number of indicators.

Nevertheless, all mandatory key features for REIs are rated with the highest marks (cf. section 2.2.3), demonstrating the suitability of the indicators for the real-time monitoring and optimization of the batch reactor.

4.2.3 Pareto-optimization

The DSS is supposed to aid in the selection of an operating mode among the set of Pareto-optimal solutions. Thus, it is necessary to obtain the Pareto-set by solving a multi-dimensional optimization problem. Equations 4.15 present the optimization problem for a single batch with length $t_f = 1500s$. The solution is the surface of the feasible region towards improved objectives. Practically, it is approximated by a set of optimal operating points with respect to the indicators defined in section 4.2.2. The Pareto frontier is obtained by off-line optimization using the CVP approach (see section 4.1.2) with six time intervals and piecewise-constant control inputs. The process constraints on all variables are enforced by path constraints every $25s$ of simulation time. The solution to the resulting NLP is obtained with the NPSOL solver of the MATLAB®/TOMLAB optimization package.

$$\min_{F_{B,in,j},Q_{trans,j}} \quad (-TME, -TEE, -ECO, -BEN) \tag{4.15a}$$

$$s.t. \quad \text{model equations} \quad 4.7a - 6.2 \tag{4.15b}$$

$$\text{process constraints} \quad 4.10a - 4.10e \tag{4.15c}$$

$$F_{B,in,j}, Q_{trans,j} \in \mathbb{R} \quad \text{for} \quad j = 1, ..., 6 \tag{4.15d}$$

The Pareto frontier describes the trade-offs that are present between the objectives, represented here by the four considered indicators. Solving the optimization problem for each objective individually yields the extreme points of the frontier listed in table 4.2. The individual optima are not necessarily unique and hence might not be on the Pareto frontier. To obtain the extreme points of the Pareto-frontier, the objective function is formulated according to eq. 4.16 and solved four times. Each time one indicator receives a weight of $w_i = 0.99$ and 0.003 on the other objectives. The small weights on the remaining objectives are necessary to find the Pareto-optimal solution in case the optimum on the main indicator is not unique and exists with worse values of the other objectives.

Table 4.2: Objective function values for individually optimized objectives BEN, TME, TEE, and ECO. The highest and lowest scores delimiting the Pareto frontier are highlighted in bold-face.

Optimized REI	BEN value	TME value	TEE value	ECO value
BEN	**3396.8**	0.616609	0.0046649	3.6878
TME	3385.1	**0.620536**	0.0028648	**3.2919**
TEE	2722.6	0.500078	**0.0074788**	9.2946
ECO	**-743.28**	**0.030061**	**1.9556E-04**	**768.96**

Optimal process operation is achieved by performing on the Pareto front. Where exactly to operate, however, is a managerial decision. The decision making process is strongly dependent on the form of the frontier, e.g. the motivation to improve the energy efficiency is higher if there is only a slight reduction of the associated benefit. The DSS should enable the user to explore the shape of the frontier. To accurately reflect the trade-offs and to enable the user to smoothly navigate on the Pareto frontier, it is necessary to obtain a set of solutions that is evenly distributed and reflects the frontier in a high resolution. The set of solutions is then recorded, together with the corresponding process inputs. Based on the users input, the set can be filtered to find the desired operating mode.

$$\min_{F_{B,in,j},Q_{trans,j}} \quad -\left(w_1 TME + w_2 TEE + w_3 ECO + w_4 BEN\right) \tag{4.16a}$$

$$s.t. \quad \sum_{i=1}^{4} w_i = 1 \tag{4.16b}$$

$$\text{model equations} \quad 4.7a - 6.2 \tag{4.16c}$$

$$\text{process constraints} \quad 4.10a - 4.10e \tag{4.16d}$$

$$F_{B,in,j}, Q_{trans,j} \in \mathbb{R} \quad \text{for} \quad j = 1, ..., 6 \tag{4.16e}$$

Each combination of weights leads to a different point on the Pareto frontier. However, the distribution of points is strongly dependent on the shape of the frontier. In case the solution space is non-convex with a concave Pareto front, the method fails entirely. In such cases, the method obtains only solutions on the edge of the hyperplane, because in combination with the linear objective function in eq. 4.16a higher cost function values are obtained there. This behavior was observed for the WOSBR application case, which indicates that the solution space is indeed non-convex. The normalized normal constraint method (NNC) was used to overcome the problem of non-convexity. As outlined in section 4.1.3, the NNC method can be used to introduce additional constraints on the objectives to obtain well distributed Pareto optimal solutions.

Application of normalized normal constraint method

Good decision support requires the possibility of a smooth navigation on the Pareto frontier without inconsistencies and discontinuities. This is achieved by a high density of Pareto-optimal points that cover all areas of the front to reflect the entire variety of possible decisions. The idea of the NNC method is to introduce additional inequality constraints that cut off parts of the feasible region, while only one objective remains in the cost function of the optimization problem. The objective and the orientation of the constrains are selected to make sure that the optimal solution will be at the intersection of the NNC constraints with the Pareto frontier. By shifting the position of the constraints the frontier can be systematically scanned. As outlined in section 4.1.3 the constraints are defined according to the following requirements: (1) being perpendicular to each other and the utopia hyperplane, which is spanned by the individual optima (anchor points) listed in tab. 4.2 and (2) intersecting with the utopia plane in utopia points that were determined by an evenly distributed grid. The number of Pareto optimal points can be increased by the number of discretization points on the utopia hyperplane. In practice however, some regions of the Pareto frontier were less densely covered or even cut off. The following challenges were identified and overcome to efficiently achieve the desired coverage:

Nonlinear boundary of the Pareto frontier

The NNC algorithm generates Pareto optimal points by introducing additional constraints orthogonal to the utopia hyperplane that is spanned by the anchor points. Thus, the generated solutions are in fact the orthogonal projection of the points on the Pareto frontier. If the boundary of the Pareto front is non-linear and extends to the outside, the projection will not yield points in this area. In this case, the area in question will not be explored, since the additional constraints on the REIs remove the corresponding solution space. In order to ensure good coverage of the entire Pareto front, the utopia hyperplane that is defined by the anchor points must be enlarged to entirely enclose the complete Pareto frontier.

The expansion of the utopia plane comes at the cost of a reduced number of Pareto solutions, because a higher fraction of the subproblems become either infeasible or their respective optimum is not a Pareto optimal solution to the global problem. Furthermore, the expansion increases the distance between the utopia points and subsequently also of the Pareto solutions. These effects can be compensated by a larger number of points at the cost of a higher computational effort.

Exact identification of the boundary

By introducing the additional constraints, individual subproblems are defined for each utopia point. The success of the run is dependent on the orientation of the hyperplane and thus the orientation of the orthogonal constraints as well as the objective selected to remain in the cost function, according to the NNC method. Since only one of the four objectives is considered, all Pareto points are oriented towards the direction of the improvement of this objective. Thus, the frontier towards the other directions is not found. By alternating the objective that is remaining in the cost function the entire boundary can be identified reliably. This approach further increases the computational effort invested into obtaining the Pareto frontier, but since the set of Pareto-optimal points is obtained offline increasing optimization times are not critical.

Computational effort

The previous two paragraphs outline the need for an increased number of optimization problems to generate a good coverage of the frontier. It is relatively easy to find a feasible solution to the given problem by choosing random sets of inputs. Since it is very unlikely that they are close to the optimum, lengthy optimization times are observed. The times can be reduced by initialization with a feasible solution close to the optimum that was obtained before. In order to obtain a good set of initial inputs for this purpose, the solution space was randomly sampled and simulated. Infeasible solutions were discarded to obtain a clean set of feasible solutions, as is displayed in figure 4.6. Then, for each NNC subproblem the set of points is reduced by the additional constraints, which are currently active. Subsequently, the best solution regarding the current cost function is used for the initialization. The computational effort per run is reduced significantly to approximately $2 - 60s$ per run.

The cloud of points represents a first estimate of the feasible region, which indeed confirms the non-convexity of the problem. The group of points shown in light gray were obtained by discretization steps on the feed rate, between 0 and $5.784\frac{kg}{s}$ for each of the six time intervals, while applying discretization steps on the interval $[-600kW, 800kW]$ for heating or cooling respectively. The group of points depicted in black was obtained with tighter constraints on the heating or colling duty. Thus, less heating and cooling energy is used, resulting in a better performance regarding the energy efficiency TEE. Figure 4.6 shows the collection of $54,297$ feasible points. Towards the optimum for the ECO indicator, the values for TEE and TME deteriorate and show a strong trade-off between the ECO performance and the other two REIs. For simplicity, the BEN indicator information is not shown in this plot.

Results

The NNC Pareto optimization, based on the discretization proposed above, yielded $13,942$ Pareto optimal points after the application of Pareto filter. Figure 4.7c shows the points obtained as a grid, where each intersection point is one solution. The graphs 4.7a–4.7b depict the Pareto frontier as a surface plot together with the randomly created solutions that approximate the feasible solution space of the optimization problem. The indicators values for TME, TEE, and ECO are recorded on the axes, whereas the benefit BEN is color-encoded.

In order to improve the interpretability, the unrelated optima for each objective are plotted in conjunction with the Pareto front in figure 4.7d. A direct linear connection between the ECO optima and any of the remaining points is located outside of the feasible solution space. Thus, the suspicion of non-convexity stated earlier is proven to be correct and delivers an explanation for the failure of the simple linear scalarization

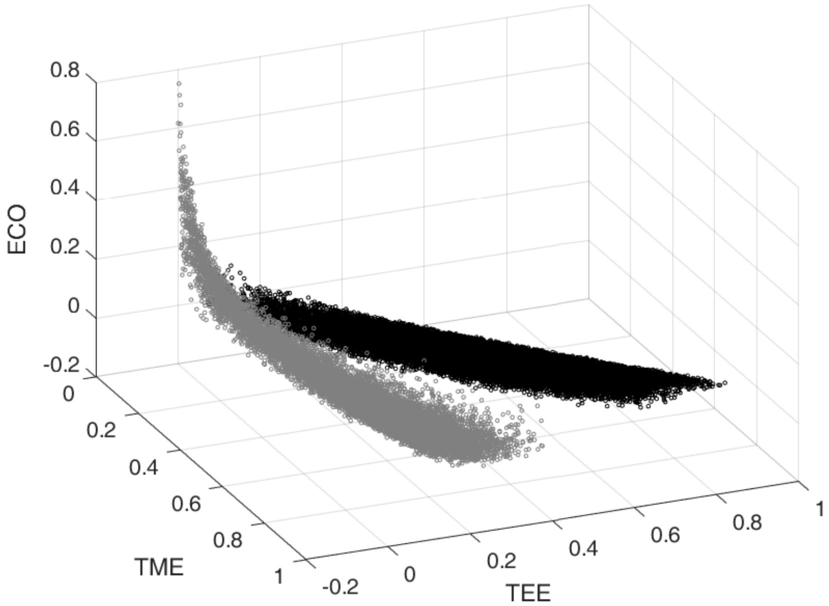
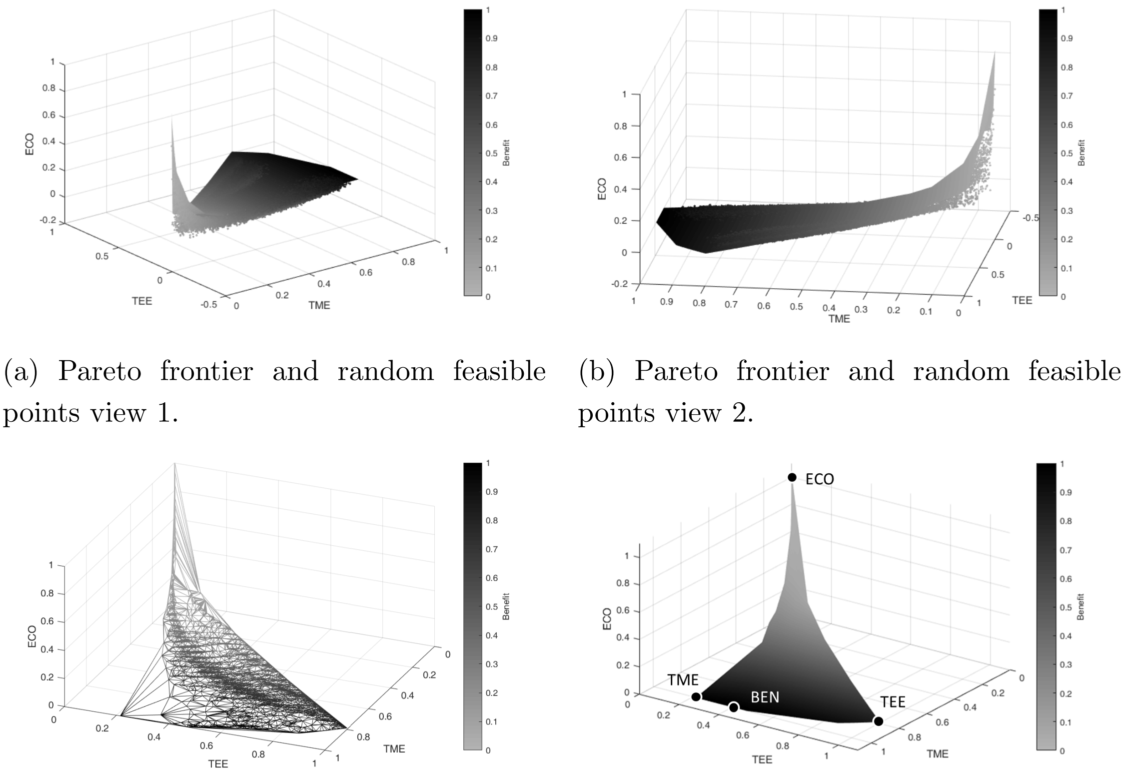


Figure 4.6: Randomly generated solutions to the global optimization problem of one batch of the WOSBR. Indicator values are scaled between zero and one. The light gray points result from the full permitted input space. The black points are the result from tight constraints on the heating and cooling, with better energy efficiency (TEE).

approach outlined before (c.f. eq. 4.16). Due to the linear cost function, the optima will either be on the ECO optima or on the line through the other three individual optima.

The form of the frontier in connection with the location of the individual optima allows for a qualitative interpretation of the optimization problem at hand. Operating points that exhibit a good ECO efficiency are only possible at the expense of large deterioration of the other three indicators. This is consistent with the observations in 4.2, where the minimal, thus worst, value of the remaining indicators is observed for the highest ECO efficiency. From an economical point of view, it is not sensible to operate the process in an eco-efficient way, since the benefit assumes a negative value. The benefit optimum is located in between the most energy (TEE) and material efficient (TME) operating points and represents the financially weighted trade-off between improved product proceeds and utility costs. The fact that the economic optimum is close to the most material efficient operating point further indicates that the benefit is dominated by the material efficiency.

Figure 4.8 illustrates the projections of the feasible region in all coordinate planes. The top-left graph confirms a strong correlation between the TME and the benefit, which is explained by the significantly higher prices for raw materials and products compared to the utility prices as listed in table A.2 in appendix A. Thus, there is no trade-off between



(a) Pareto frontier and random feasible points view 1.

(b) Pareto frontier and random feasible points view 2.

(c) Grid of Pareto optimal points.

(d) Pareto frontier with utopia points.

Figure 4.7: Representations of the Pareto front and feasible operation points. The indicator values are scaled with respect to the best and worst values identified in table 4.2.

the material efficiency and benefit (BEN). The correlation between TEE and BEN, as well as TEE and TME is less pronounced. Considering the top-right and center-right graph in fig. 4.8, operating points can be found that achieve different energy efficiencies for a given benefit or total material efficiency. In principal, two explanations seem plausible for this behavior: (1) either the influence of heating and cooling onto the benefit and reaction yield is negligible or (2) the dynamic nature of the production allows for different temperature and concentration trajectories that result in the same BEN and TME with different usages of utilities. Bearing in mind the positive direction of improvement, the remaining three graphs under participation of the ECO indicator are another confirmation of the non-convexity property of the optimization problem that requires the usage of the NNC method.

Solution structure

The input structure and resulting batch trajectories are considerably different for the individual optima. To elucidate the differences and cause-effect relationships, the batch trajectories for the optima are shown in figures 4.9–4.13. The decision variables for each batch are the heating and cooling rate, as well as the feed rate of raw material

B that are step-wise constant in six time steps of $250s$. The heating and cooling rates are directly plotted over the batch time at the top-left of each figure, influencing the temperature trajectory shown at the top-right. The feed rate of raw material B is implicitly shown as the growing reactor content in the lower left graph in addition to the pre-charged raw material A with $V_R = 2m^3$ at $t = 0$. The transfered energy is constrained between $+800kW$ heating and $-600kW$ cooling, whereas the maximum feed rate is $5.784kg/s$ of B. In addition, the maximum reactor volume and the temperature constraints are indicated by dashed lines. The trajectories in the lower-right graph track the reactor content regarding the intermediate and final products in kg. Here, the only relevant constraint is the requirement of at least $50kg$ of product P at the end of the batch.

Figure 4.9 shows the results for the most energy efficient operation which is measured by TEE according to eq. 4.12. The TEE improves for an increased amount of the products P and E or a reduced amount of cooling and heating. As a result of the indicator definition and the optimization efforts, the heating and cooling duty is reduced to zero. Consequently, the batch executes adiabatically after introducing the raw material B. The

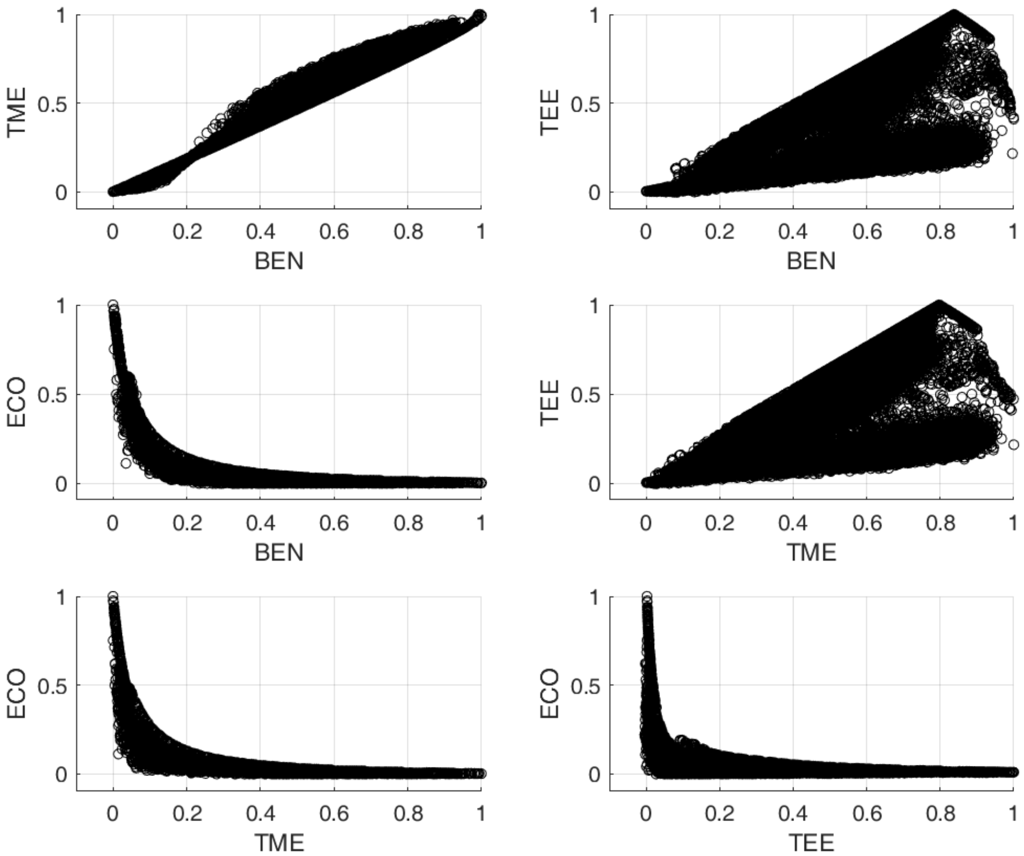


Figure 4.8: Projections of all feasible solutions into the different indicator planes.

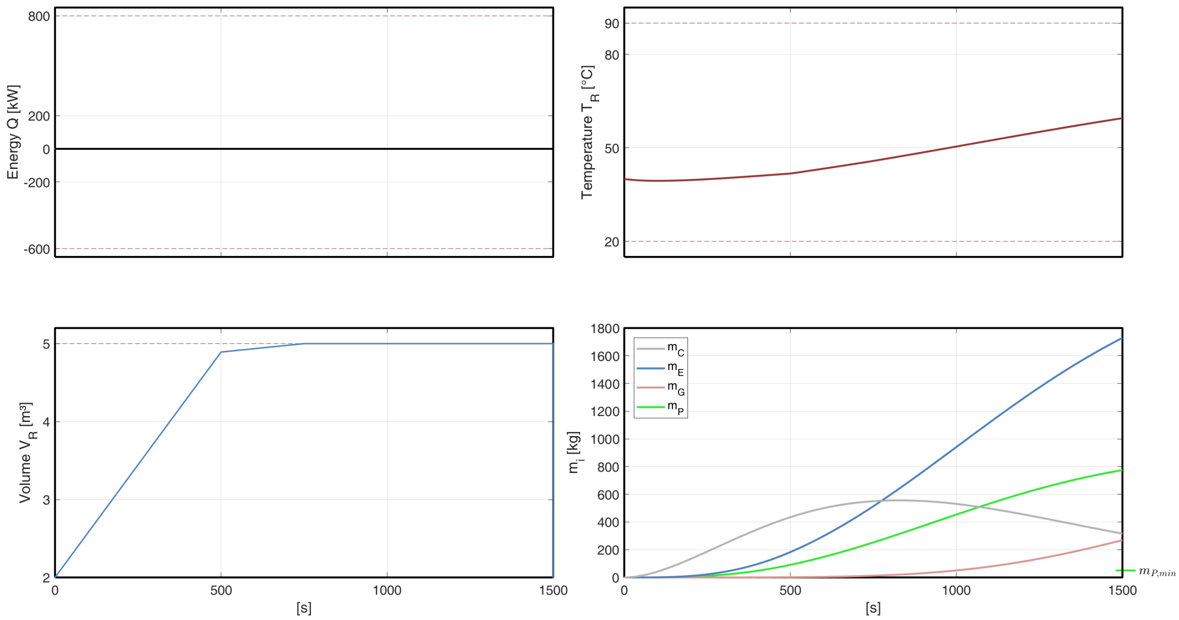


Figure 4.9: Batch trajectories for optimal energy efficiency (TEE).

temperature trajectory develops solely as a result of the feed temperature of $35°C$ and the three exothermic reactions initiated in the reactor. At the start of the batch, the concentration of raw material B is small and the heat effect due to reaction is negligible. Thus, the cooling effect of the feed is dominant, leading to a slight reduction of the rector temperature. With an increasing amount of raw material B the first reaction yields an increasing amount of intermediate product C according to eq. 4.4 (c.f. gray trajectory in fig. 4.9, bottom-right). In the further course of the batch, the other two reactions begin to yield the products P (green), E (blue), as well as the undesired co-product G (red). Simultaneously, the heat of reaction starts to compensates the cooling effect of the feed. This leads to an increase of the reactor temperature, accelerating all reactions. The accelerated reaction also increases the amount of products, positively influencing the TEE indicator. In order to maximize the product formation, the raw material B is introduced as early as possible to increase the available reaction time in relation to the fixed batch length.

Figure 4.10 shows the results for the most eco-efficient operation, measured by the ECO indicator according to eq. 4.13. The indicator improves for an increased amount of the products P and E or a reduced amount of toxic product G at the end of the batch. Thus, the objective is to maximize the yield of reaction equation 4.5 relative to yield of reaction equation 4.6, while fulfilling the endpoint constraint of at least $50kg$ of product P. This is achieved by an operational strategy minimizing the reactor temperature and the introduction of raw material B as late as possible. The reactor temperature directly influences all reaction rates via the Arrhenius equation (eq. 4.8e) to a different degree.

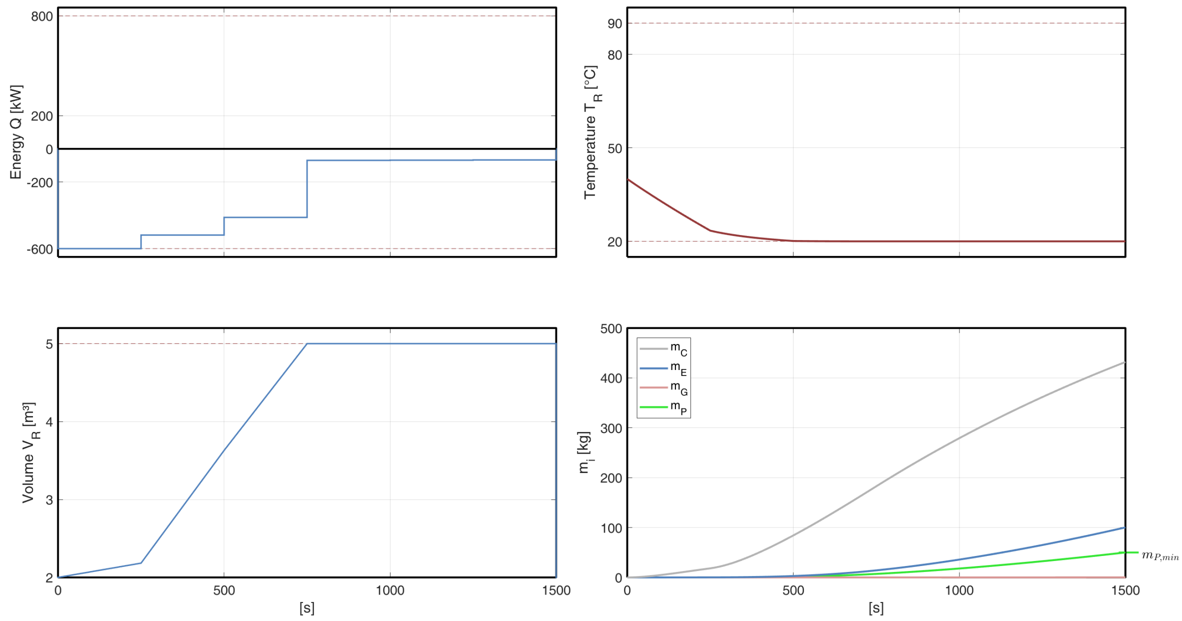


Figure 4.10: Batch trajectories for optimal ECO efficiency.

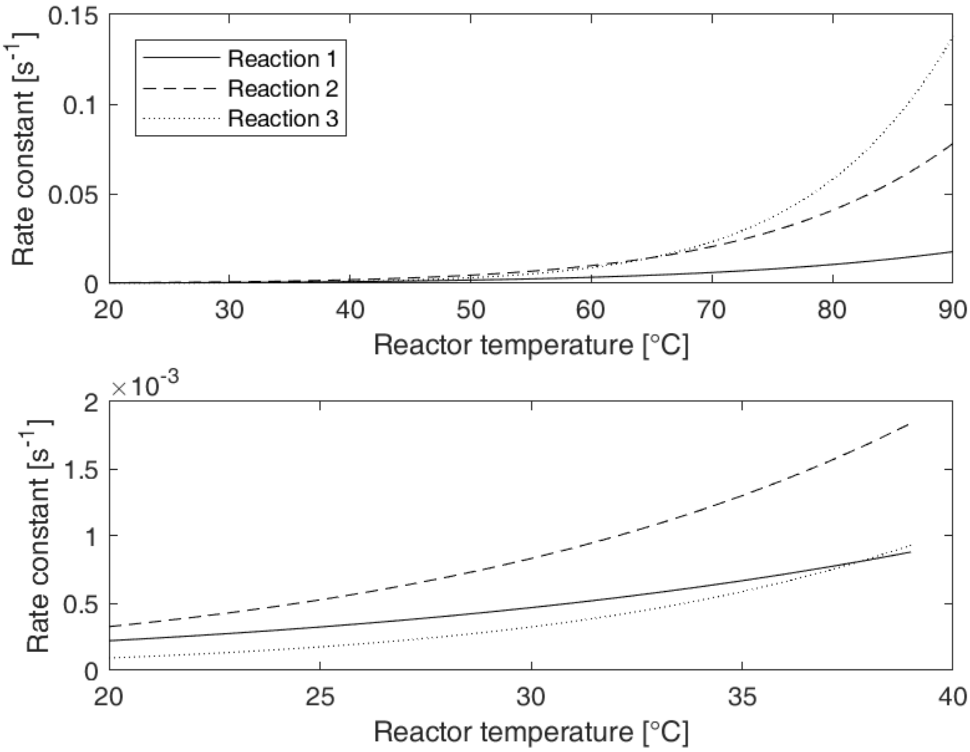


Figure 4.11: Temperature dependency of Arrhenius rate constants for the reactions eq. 4.4-4.6. Top: the entire permitted temperature range. Bottom: partial temperature window for better readability.

Figure 4.11 shows the temperature dependent reaction rate constants r_1, r_2, and r_3 within the permitted reactor temperature range. For temperatures below $38°C$, the rate constants of reaction one and two are higher than the undesired reaction three that involves the formation of the eco-efficiency relevant species G. For temperatures at the high end of the permitted range, the reaction rate constant of reaction three grows significantly faster than the others, strongly favoring the decomposition of valuable products to the undesired co-product G. Thus, the optimal trajectories in fig. 4.10 are achieved by operating the reactor at the lower temperature constraint. Here, the rate constant ratios r_3/r_1 and r_3/r_2 are minimal. The second effect that is beneficial to the ECO indicator value is to introduce the raw material B later to reduce the reaction time that is available for the unwanted side reaction. In comparison to the energy efficient operation in fig. 4.9 the feed profile of B is shifted to the right, but still rather early in the batch, which is due to endpoint constraint on P that needs to be met. This combination of process trajectories results in the optimal ratio between the products P/E and the component G. The overall product yield is significantly smaller than at the most energy efficient operation due to the low reaction temperature, while investing the maximum amount of raw material B and a significant amount of cooling. Thus, the eco-efficient production results in the worst Pareto-optimal values regarding the other REIs.

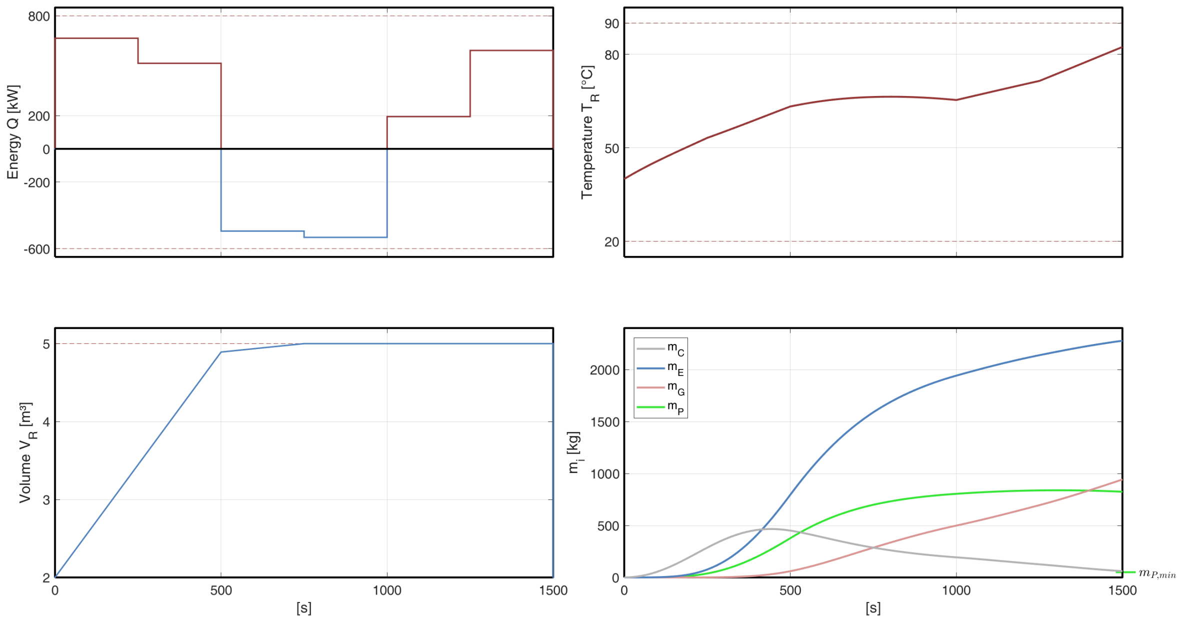


Figure 4.12: Batch trajectories for optimal material efficiency (TME).

The total material efficiency indicator (TME) is defined according to eq. 4.11 and relates the amount of product to the invested raw material. Raw material A is pre-charged completely before the start of the batch, thus the material efficiency is only determined by the amount of B fed and the obtained content of the products. Similar to the case of energy efficient operation the available reaction time is maximized by early addition of raw material B to maximize the product formation (c.f. 4.12, bottom-left). The optimal heating and cooling input is displayed in the upper-left graph. It is characterized by heating at the beginning and end of the batch, whereas cooling is applied in the middle of the batch between $500s$ and $1000s$. The initial heating compensates the effect of adding the sub-cooled feed, which leads to an accelerated production of the intermediate C. The fast formation of the intermediate product is the prerequisite for an early start of the second, product forming, reaction. Cooling during the middle phase compensates the heat introduced by the exothermic reactions, resulting in a constant reactor temperature around $65°C$. Considering the observations obtained from fig. 4.11 it is plausible to assume that the temperature is limited here to limit the reaction rate of the product degenerating side reaction. Towards the end of the batch the reactor is heated again, which increases the reaction rates of reaction 4.5 and 4.6. Due to the time constants of the system, reaction 4.6 is delayed and finally interrupted by the completion of the batch. This limits the amount of degradation regarding product P and results in optimal material efficiency.

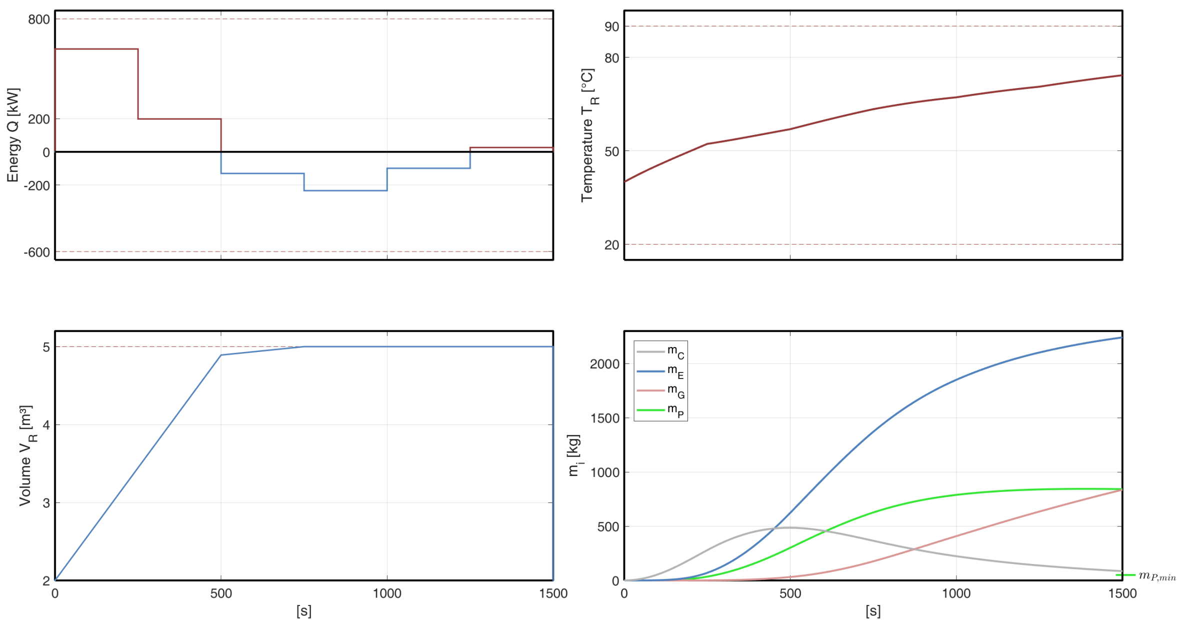


Figure 4.13: Batch trajectories for optimal benefit (BEN).

The BEN indicator captures the economic performance of the production after eq. 4.14 by summation of all relevant cost contributions. Positively contributing are

- proceeds of the products P and E at the end of the batch c_{prod} and
- proceeds c_{inc} from the incineration of intermediate product C.

Furthermore, the benefit is reduced by

- costs for the raw materials $c_{raw,A}$ and $c_{raw,B}$,
- utility costs for heating c_{heat} and cooling c_{cool} and
- the disposal costs c_{toxic} for the toxic component G.

The most economic operation is achieved by balancing the trade-off between positive and negative contributions to the benefit. The resource efficiency indicators TEE, TME, ECO, as well as the benefit are improving for an increased amount of product. Furthermore, the varying operating policies are affecting the negatively contributing factors utility usage, raw material consumption, and formation of G. Table 4.3 gives an overview of the absolute cost contributions for all four individual optima. The most significant contributions are the raw material expenditures and product revenues of P and E, where the raw materials contribute equally in all four cases. The influences due to the incineration of C, the disposal of G and utility costs are negligible, thus the overall benefit is decided by the final product yield alone. A comparison of the input trajectories indicates that the most economically viable operation is a compromise between the TEE and TME optimal operation. Factoring in the observations regarding tab. 4.3 it becomes apparent that the trade-off is not between utility cost and product revenue, but rather an optimization of the ratio between the two differently priced products.

Table 4.3: Cost and revenue contributions to the overall Benefit (BEN) for the optimum for each indicator.

Optimized variable:	BEN	TME	TEE	ECO
Cost A	-301.72	-301.72	-301.72	-301.72
Cost B	-678.88	-678.88	-678.88	-678.88
Revenue C	3.75	2.64	13.82	18.89
Revenue E	2535.77	2577.36	1956.45	113.42
Disposal G	-63.06	-71.09	-20.32	-0.01
Revenue P	1905.17	1866.43	1753.25	113.28
Cost cooling	-2.20	-4.89	0.00	-8.26
Cost heating	-2.00	-4.67	0.00	0.00
Overall Benefit	3396.83	3385.17	2722.60	-743.28

Other solutions on the Pareto frontier are intermediate steps that are gradual shifts between the extreme solutions. In order to enable a broad user group to navigate on the Pareto front, an efficient human machine interface is necessary that supplies decision support according to the intended operational targets. From the economical point of view the operating point with optimal benefit is preferable and the optimal feed and temperature trajectories are available from the stated optimization results. In case additional targets regarding the resource efficiency are considered, a preferable operating point can be selected among the set of Pareto-optimal points.

4.3 Conclusions

The framework for the definition of resource efficiency indicators developed in Chapter 3 was applied to the Williams-Otto semi-batch reactor benchmark process that was published by Williams and Otto (1960); Ebrahim et al. (2016). The final product composition is influenced by the feed profile of component B, the heating and cooling duty, and the system dynamics. The resulting resource efficiency was captured with indicators for the total energy efficiency (TEE), the total material efficiency (TME), and the eco-efficiency (ECO). In combination with the economic benefit (BEN), a four dimensional optimization problem resulted that was solved using the NNC method. The set of Pareto-optimal operating points reflects the trade-offs between competing objectives. The degrees of freedom of the process are the timing and amount of raw material B added and the heating and cooling profiles. To solve the optimization problem efficiently, the inputs were approximated as piecewise constant to formulate the problem as NLP. By using the NNC method, a sufficiently good resolution of the Pareto front could be achieved. For each of the points on the front, the corresponding inputs are known and are available for decision support. This is the main advantage of a model-based approach: It is possible to find the Pareto optimal operating points before the plant was operated at these points. The WOSBR is an interesting object of study, since the individual optima differ in their structure, resulting in trade-offs. In a real industrial application, of course, process variations occur that cannot be fully represented by the model. However, in order to make good predictions, the model must represent all relevant influences as far as possible. In addition, aging processes of the plant can lead to a changed behavior. This is called plant model mismatch and can be corrected by regular adaptation of the model parameters. Individual model parameters can be optimized with respect to the plant behavior of the near past.

By knowing the Pareto front and the associated process inputs, the manager of a plant or plant section can select an operating point on the Pareto front that meets his requirements. The associated inputs can then be used in the next batch. Since this is a complex multidimensional Pareto front, its representation is not trivial and requires a well-designed human machine interface. This task will be tackled in the following chapters.

Chapter 5

Visualization and decision support

The decision-making process to select an operating point is difficult. The various resource efficiency indicators and associated costs must be weighed against each other, while at the same time taking into account all relevant constraints that limit the process window. These include, for example, safety limits and the interaction with other plant components. By pre-processing the required information to summaries and exceptions the necessary amount of reasoning by the user is reduced during the interaction. Thus, the interface should be specifically tailored to the concrete task to provide the most efficient and effective decision support (Kalliski et al., 2018). First, section 5.1 summarizes general design concepts for human machine interfaces from literature. Then, section 5.2 screens the most common visualization elements for their suitability in multi-dimensional decision support and gives guidance on the selection of suitable elements based on characteristics of the intended application. Section 5.3 derives a design methodology to compose decision support systems for resource efficiency optimization in the process industry. The design method aims to implement a system that is simple and easy to use in order to reduce error rates and to increase user-friendliness. Finally, the design method is applied to the WOSBR application case in section 5.4

5.1 State-of-the-art

High quality decision support requires a tailored decision support solution, the design of which specifically addresses the intended decision making process to support the user. The objective is to process and deliver the required information for easy interpretation and fulfill the relevant process constraints. The skill, rule and knowledge framework outlined in section 5.1.1 is the basis for the ecological interface design (section 5.1.2) that delivers a framework to support the design process of the decision support solution.

5.1.1 Skill, rule and knowledge framework

The behavior of skilled process operators can be classified into three different layers, according to Rasmussen (1983). The direct interaction takes place on the *skill-based* level, where sensori-motor patterns are used to apply actions to the process by the manipulation of process variables (see Fig. 5.1). The action is either triggered directly on the *skill-based* level by a reflex as a response to a sensory input or on the *rule-based* level according to an existing rule. *Skill-based* operator behavior is executed with little to no cognitive load, but is hardly observed in decision making processes in the control room environment. The *rule-based* execution of tasks involves more cognitive capacities, because perceived signs need to be associated with a preexisting rule. For situations that cannot directly be associated with a known state-rule pair, a new rule must be designed on the *knowledge-based* level. Here, the situation is evaluated using a mental model or simulations of the process to trigger the subsequent decision making and planning process under consideration of the goals that have to be achieved.

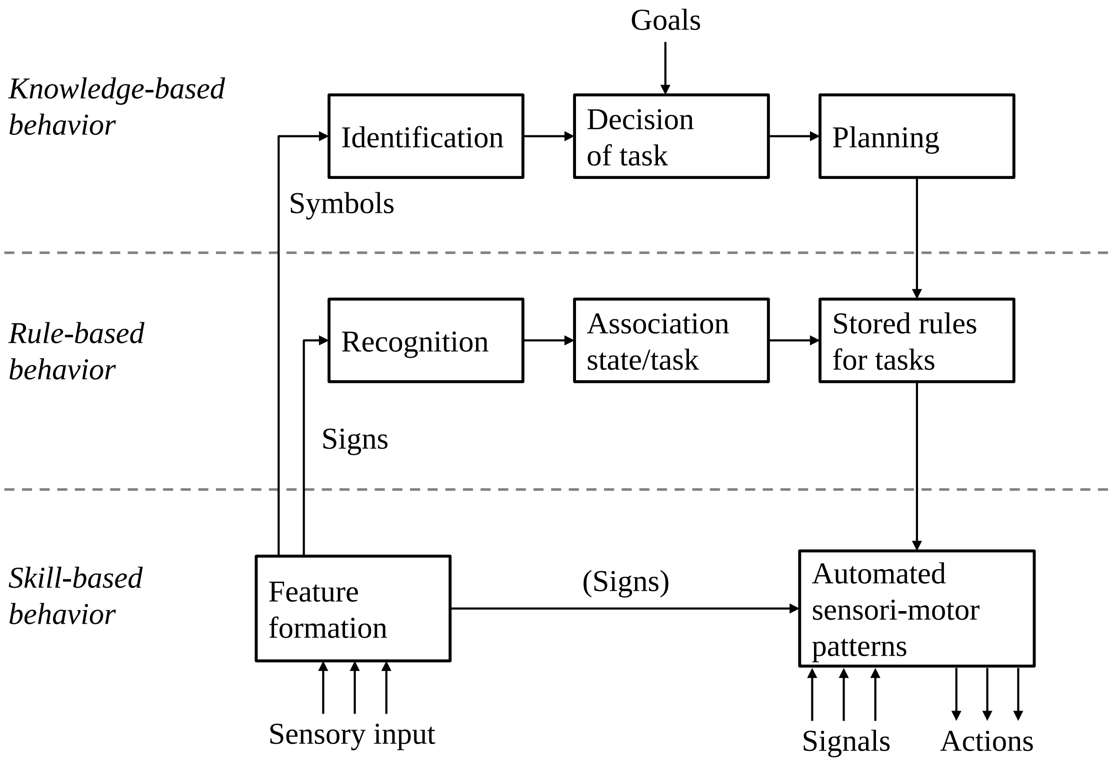


Figure 5.1: Illustration of the three levels of the performance of skilled operators. Adapted from Rasmussen (1983).

The sensory input in the control room setting is the interface that is used to display information about the process. Each level of operator behavior requires a different type of information that can either be displayed by the same or by individual visualization elements. The types of information can be differentiated into *signals, signs,* and *symbols.* Signals are measured quantities, usually as time series data that have no additional meaning other than the direct physical data. If the interpretation of a signal is dependent on other factors, the information is contextual and referred to as sign that is indicative of a specific situation that can be responded to by predefined corrective measures. In the context of causal functional reasoning or explaining unfamiliar behavior of the process, information is perceived in the form of symbols.

5.1.2 Ecological interface design

Any human-machine interface is at the interface between the user and a potentially complex system. From a structural point of view this setup extends the technical system to include the interface and the human element. The idea of an ecological interface design (EID) was first introduced by Rasmussen and Vicente (1989) with the intention to investigate multiple error classes and the implications on good interface design. The method was further developed by Vicente and Rasmussen (1992) where the theoretical foundations were summarized. An example for the application was published by Vicente and Rasmussen (1990) that is concerned with the design of an interface for a thermal-hydraulic press. Thus, EID was initially developed as an approach to minimize wrong decisions, especially for processes that are safety relevant. The observed errors were preceded by events that could be grouped in three categories:

- Familiar events that occur often. Based on the operators experience the goal can be reached with little effort if the necessary information is displayed.
- Unfamiliar, but anticipated events that occur infrequently. Operators do not encounter these events regularly, but the system designers have anticipated the situation. In principle, procedures and corrective actions are available to counter the impact of the events observed.
- Unfamiliar and unanticipated events. They rarely occur and were not foreseen by the designers. The operators cannot rely on any previously generated analysis or operating procedures. This type of events is most prone to erroneous decisions.

The design of decision support interfaces should consider all three types of adverse events. The EID framework formulates the three following prescriptive design principles, following the skill-, rule-, knowledge framework (see section 5.1.1 and (Rasmussen, 1983)).

> "**Skill based behavior (SBB)** – To support interaction via time-space signals, the operator should be able to act directly on the display, and the structure of the displayed information should be isomorphic to the part-whole structure of movements."

Skill-based decision making requires the lowest amount of cognitive effort. In most of the cases the user cannot directly act upon the technical system due to spacial restrictions and the complexity of the system. The interface should abstract functional parts of the system to a simplified representation that symbolizes the subsystem in its functional properties. If the interface is designed correctly, events that require skill-based behavior trigger a direct response based on the operators experience.

> "**Rule based behavior (RBB)** – Provide a consistent one-to-one mapping between the work domain constraints and the cues or signs provided by the interface."

For unfamiliar but anticipated events, solution strategies are available. The key to successful decision support is an efficient depiction of clues that can help to identify a relevant event. The study of incident reports (see Malone et al. (1980)) shows that it is also important to depict constraints that are relevant to the validity of the clues and signs. Otherwise, decisions based on the supplied information can be wrong and lead to undesired outcomes. Compared to skill-based decision making, rule-based considerations involve a higher level of cognitive effort (see 5.1.1). Thus, the probability for mistakes increases and interface performance is of high importance.

> "**Knowledge based behavior (KBB)** – Represent the work domain in the form of an abstraction hierarchy to serve us in an externalized mental model that will support knowledge-based problem solving."

The third category involves unfamiliar and unanticipated events. Here, the decision making process requires a high level cognitive effort, because the user needs to combine current information about the system state with a mental model of the process. The mental model includes all experience and theoretical knowledge that the user can recall. In order to create this process in the most efficient way, it necessary to supply all relevant information that is available about the system. Furthermore, the designer must have an idea about the users' experience and most probable structure of the mental model.

5.2 REI-based decision support

Section 5.2 has been published in Kalliski et al. (2018)[1].

Decision support systems (DSS) are computer-based applications that summarize and process relevant information to prepare decisions to be made by the user. Classic DSS

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include database management capabilities with access to required information, models or calculation routines and a user interface to display the information created by the system (Shim et al., 2002). DSS were first developed during theoretical studies of organizational decision making and parallel efforts, motivated from a technical point of view, during the 1960s (Keen and Scott Morton, 1978). They were initially designed to support individual decision makers in a business environment, where decisions needed to be made for specific and well-designed tasks (Alter, 1977; Keen, 1980). Later, the development shifted towards tools that refine and prepare data for complex systems and ill-structured problems that require the user's experience (Ariav and Ginzberg, 1985; Er, 1988). Since then, the scope broadened to address all sorts of decision-making processes, ranging from scheduling and production planning applications to intelligent DSS that adapt to changing production structures and constraints (Mahdavi and Shirazi, 2010). DSS include the user's expertise in the decision-making process, in contrast to "expert systems" that try to emulate human decision making. A specific form of DSS are business intelligence (BI) systems that can be seen as systems that evolved from general DSS, but focus strongly on data visualization, where modeling and deterministic reasoning are not as obvious as in technical processes.

In this thesis the term DSS is defined as a "computer-based application summarizing, relating and displaying information relevant for the human decision-making process". The design and the necessary capabilities of a DSS strongly depend on the decisions to be made and the environment in which the system is going to be operated. Despite the diverse field of applications and the continuous progress in research and application, the six-step DSS development framework of Pearson and Shim (1995) can be used as a template for the design of DSS for resource efficiency in processing industries:

(1) Identify the environment in which the DSS will be used.
(2) Ascertain the role the DSS is to have in support of the decision-making process.
(3) Identify the specific capabilities that are required to support the decision maker within the environment identified in step 1.
(4) Develop a conceptual design of the DSS.
(5) Based on the conceptual design, determine the resources required to build the DSS.
(6) Build the DSS and provide for ongoing support.

The development of DSS for resource-efficient production can be performed by customization of generic methods, designs and tools to the application case. The REIs that were defined in accordance with the guidelines presented in Chapter 3 are specifically designed to capture the resource efficiency of production processes in the processing industry and offer great potential for decision support applications. Indicators that are referenced against a baseline of the process already provide valuable decision support by providing a savings potential.

Visualization techniques are used to present data to the users in an abstracted representation that is intended to ease the interpretation process by giving meaning to data and supporting an efficient perception. The real-time REIs described in Chapter 3 are the first step to extract meaningful information from the process data. They offer the visualization of preprocessed information based on an efficiency analysis, rather than plain production data. Monitoring the resource efficiency of a plant needs to be holistic to differentiate between potentially competing contributions from environmental performance, material efficiency and energy efficiency, in order to reflect the overall resource efficiency. The task of visualizing the multidimensional entity "resource efficiency" in relation to the plant structure and production process is not trivial and calls for an efficient dashboard design to minimize the cognitive load for users in a demanding work place. Section 5.2.1 outlines general considerations about the principles of human-machine interfacing and the implications for the visualization of REIs. Sections 5.2.2 introduces suitable visualization elements and 5.2.3 give practical guidance on how to choose the correct visualization elements, based on the properties of systems.

5.2.1 Principles of human-machine interface engineering

Section 5.2.1 has been published in Kalliski et al. (2018)[2].

Few (2006) lists HMI features that help to improve their quality. Below the implications on REI-based decision support are summarized for each characteristic:

- **Exceptionally well organized**
  The representation of complex systems requires multiple REIs and supporting information; thus multiple plots and graphs are needed. Grouping in rows, columns and fields increases readability and reduces the time required to find the needed information. The reading direction of the user should be taken into account during the dashboard design process, e.g. from left to right and top to bottom for Western cultures. Taking advantage of this subconscious preference, the most important information should be displayed in the top left area and the least important information on the lower right (cf. Figure 5.2).

- **Condensed, primarily in the form of summaries and exceptions**
  Information in the form of a large number of data points is not helpful in the interpretation process. The defined REIs are in fact summaries over meaningful time scales and subsystems, making it possible to see the whole picture. Data plots showing plant behavior in the bounds of normal operations should be displayed unobtrusively with light colors and low intensity. More intense colors and forms of

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representation should dynamically occur in the case of exceptions, e.g. situations that require evaluation by or input from the operators, in order to guide the user's attention.

- **Specific to and customized for the audience and objectives**
  The information presented to the recipient should be based on what is needed to execute the task at hand. Insight into what this information is can be gained by observing the operational procedure in the current setup and through structured interviews to assess how decision are currently made.

- **Displayed using concise, often small media that communicate the data and its messages in the clearest and most direct way possible**
  The content and density of information in a visualization element should be limited to a minimum that still serves the intended purpose. This includes aspects such as background coloring, background pictures and unnecessary grids and borders. These rules were introduced as the concept of "data-ink ratio" by Tufte (2006), stipulating the reduction of elements that do not aid in the comprehension process.

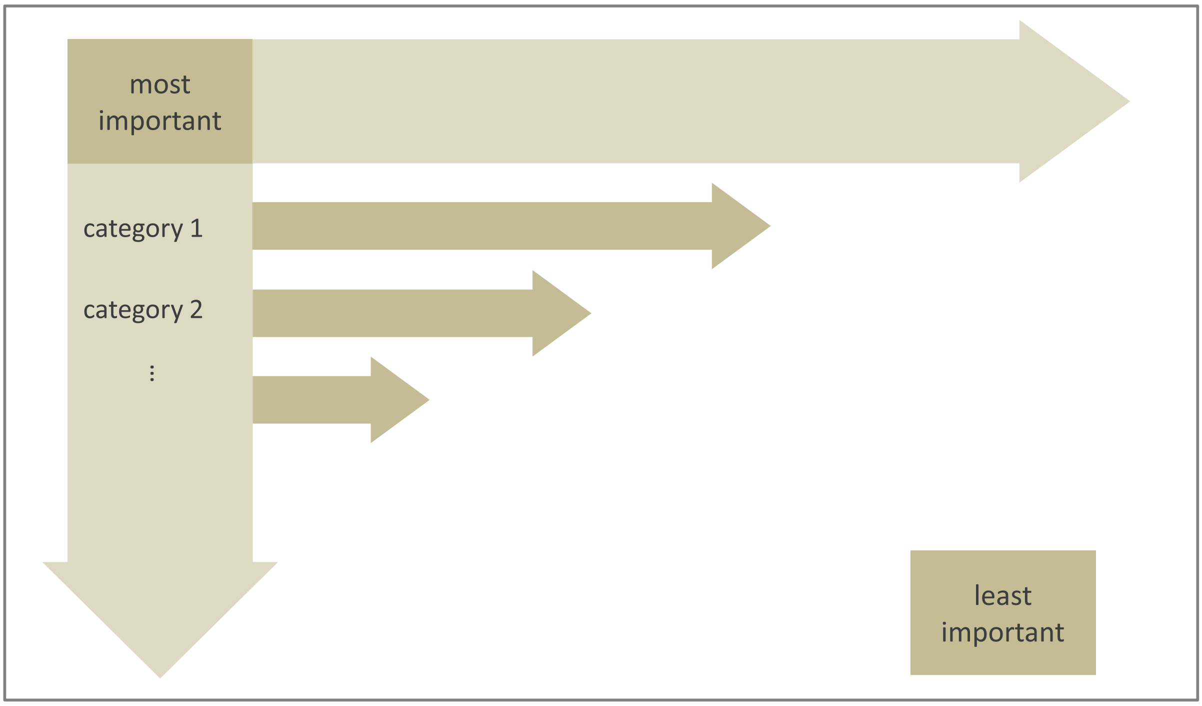


Figure 5.2: Structure of well-organized dashboard configurations for Western users.

Based on these requirements for dashboard representations, Few (2006) identified 13 common violations of these rules that should be avoided in the design of effective visualization solutions:

(1) Exceeding the boundaries of a single screen

(2) Supplying inadequate context for the data

(3) Displaying excessive detail or precision

(4) Choosing a deficient measure

(5) Choosing inappropriate display media

(6) Introducing meaningless variety

(7) Using poorly designed display media

(8) Encoding quantitative data inaccurately

(9) Arranging the data poorly

(10) Highlighting important data ineffectively or not at all

(11) Cluttering the display with useless decoration

(12) Misusing or overusing color

(13) Designing an unattractive visual display

5.2.2 REI visualization elements

The overall resource efficiency of a plant can be expressed in a set of indicators, which may be dependent or exhibit a trade-off. Thus, it is sensible to decompose the different aspects of resource efficiency into small and concise media that can be simultaneously displayed for easy perception and pattern recognition by the operator. Below, visualization elements are discussed to determine which formats are most useful for specific visualization goals. In the context of resource efficiency monitoring the objectives are

- the identification of trends,
- the monitoring of compliance with production targets,
- obtaining an overview of the process, or
- showing quantitative and qualitative aspects of resource efficiency.

Sunburst diagrams
In chemical processes raw materials and energy are consumed, whilst producing the desired product as well as material- and energy-waste streams. Sunburst diagrams (c.f. Figure 5.3) are useful to visualize the distribution of energy and materials from plant level to unit level. The visualization based on the circular design and multiple layers representing the plant hierarchy allows the user to compare shares on the same levels as well as on different

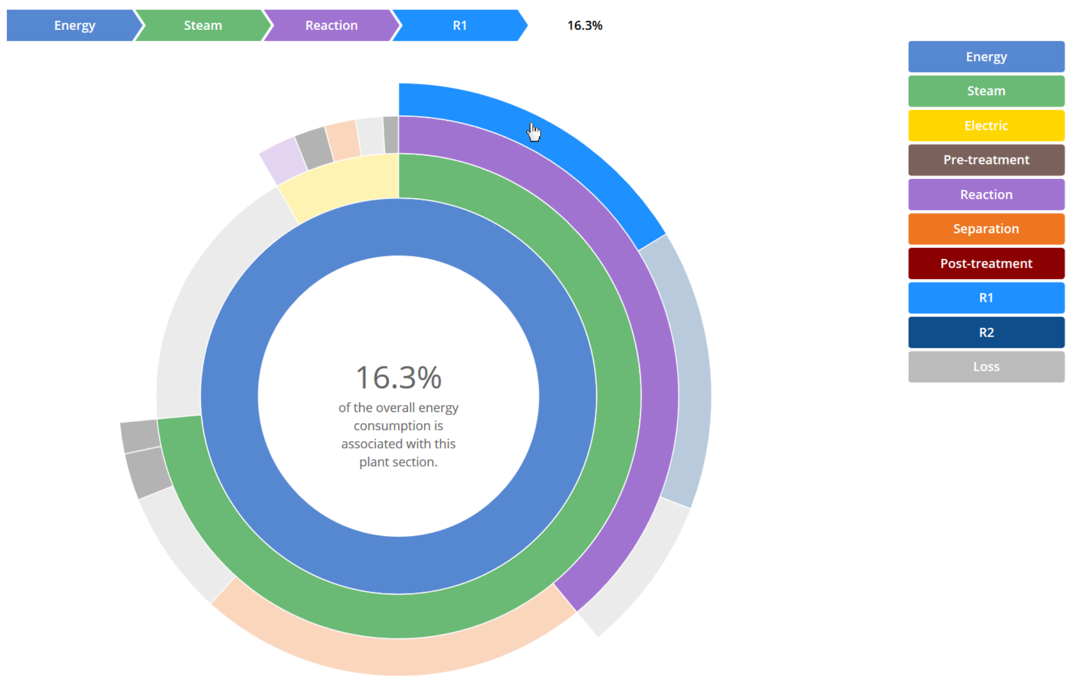


Figure 5.3: Sunburst diagram for the energy consumption by plant section. The selection of reactor R1 triggers the highlighting of the trace: Energy, Steam, Reaction to R1. The other recorded energy consumption is grayed out.

levels. Main consumers are identified effortlessly and may point out where to check for optimization potential first. Upon user input the category of interest and the trail from the highest level (center of the circle) is highlighted, supported by the display of the numerical value shown in the middle of the diagram. Additionally, the trail of categories is shown on the top left corner, which minimizes the need to consult the legend on the right of the diagram. This visualization technique is most suited to give an overview of the energy consumption on an energy or site management level but is too coarse to derive operational actions from.

Indicators included in plant structure

Generic REIs are defined for functional units of the plant and can be aggregated to obtain the efficiency of plant sections or the entire production site. The tendency of operators and engineers to think in terms of the process and its structure can be exploited by introducing bar scales to the flow diagram of the plant setup, summarizing the resource efficiency of the unit. Thus, the user is able to assess the resource efficiency performance of the sections at a single glance (cf. Figure 5.4).

If the indicator value of a section drops below a minimal target value, the section is highlighted by a darker shade of gray and the bar will change the color from dark gray to a light color. It will start flashing for very low values to highlight the suboptimal operation to the staff.

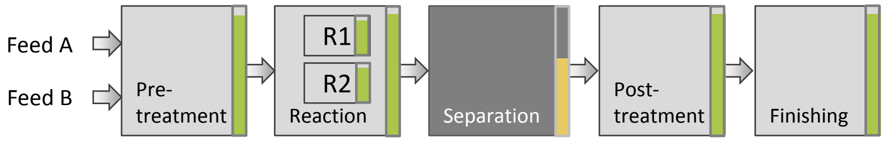


Figure 5.4: Structure of well-organized dashboard configurations for Western users.

Sankey diagrams abstract a given plant structure and visualize the pathway of material and energy through the system. Figure 5.5a shows two raw materials being fed to a reactor yielding a mixture of the product with impurities that is fed into the consecutive separation stage where the mixture is split into the pure product and the waste material.

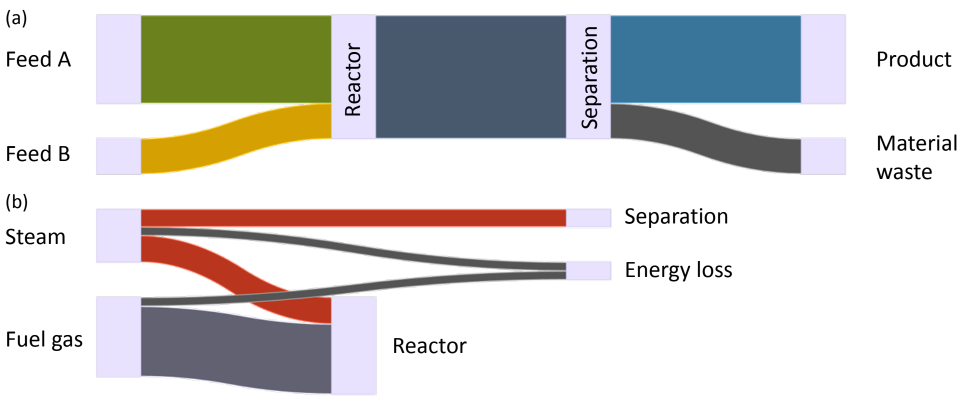


Figure 5.5: Sankey diagram for materials (a) and energy (b).

The second plant structure in Figure 5.5b shows the flow of energy into the reaction and separation steps, as well as the associated losses. Sankey diagrams are suited to visualize the paths of materials and energy through the plant structure for simple to medium-complex systems and pathways. They are useful to identify the most important streams and the key equipment to be analyzed for resource efficiency. Upon user interaction the selected streams are highlighted by introducing transparency to the rest of the diagram, while displaying the current flow rate and the theoretical minimum necessary to achieve the same amount of product (cf. Figure 5.6). This visualization technique is suitable to track mass and energy flows through the plant for a detailed analysis during resource efficiency projects, but it is usually too complex for the operational personnel in day-to-day operations.

Radar plots

Figure 5.7 shows radar plots for five indicators that were referenced against a theoretical or historical optimum, thus they can adopt values between 0 (poor efficiency) and 1 (perfect

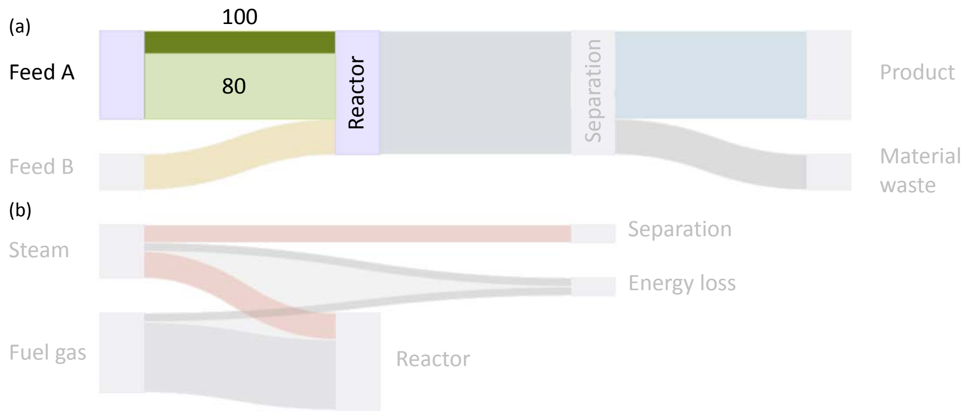


Figure 5.6: Sankey diagram with highlighted raw material feed A with a measured flow rate of $100kg/min$ and a theoretical minimum of $80kg/min$.

efficiency). The light brown area depicts a performance below an individual target. As long as all indicators are above the target, the system is considered to be well operated. The target threshold differs from case to case and needs to be carefully defined by the plant management specifying the dashboard. The plot on the top shows a static version that is useful to obtain a fast overview about the process at one glance. The lower radar plot in Figure 5.7 is a dynamic radar plot that indicates the current situation with a black line and previous configurations in gray, where lower intensities stand for values further in the past. This is especially useful for batch processes. This visualization concept is very well suited for the verification of compliance with targets and can be broadly used to show qualitative tendencies. The minimal number of indicators required to produce a radar plot is three, being theoretically unbound for the maximal number of REIs to be shown. Practically the interpretation of the plot becomes ambiguous for significantly more than five REIs.

Bullet Chart

Figure 5.8 shows a bullet chart that conveys highly condensed information about the current indicator value against a target value, the historical variation and the predicted trend as an extrapolation. Here, the scale is chosen with respect to a theoretical optimum or best achieved value (100%). The white interval of the scale indicates the target performance, and the gray interval an undesired operational state. The lower bound of the scale should be chosen as 0% to achieve a consistent and comprehensible visualization. In case the desired domain of operation is very close to the optimum, it is useful to choose a higher value as lower bound for the scale to secure a reasonable resolution. Triangles are used to mark the current value and are complemented with the numerical value on the opposite side of the bar and an arrow designating the direction of movement based on the extrapolation of the current trend. The rectangle on the left side of each bar shows the variability of the indicator in the near past. In case the indicator leaves the desired

Figure 5.7: Static (top) and dynamic (bottom) radar plot for selected indicators.

operational interval, an exception occurs that is emphasized by a change in color of the variance interval and the appearance of a caution sign above the scale. The history of the indicator is stored implicitly in the size and position of the variability bar, the current position relative to the variability bar and the arrow indicating the direction of movement. If the plant operates stably within the desired efficiency range, the variability bar is small and lies entirely in the white area. A plant upset manifests itself in large variability bars that may reach into the sub-target range. A triangle position at the border of the variability bar in combination with an arrow pointing further away from the variability bar indicates a transient trend away from the former average, which can be an early indicator for the operator to intervene and take corrective measures. Finally, the change of color and warning signal draw the users' attention to the state. Bullet charts do not necessarily have to be oriented from bottom to top, but can also be displayed from top to bottom (in

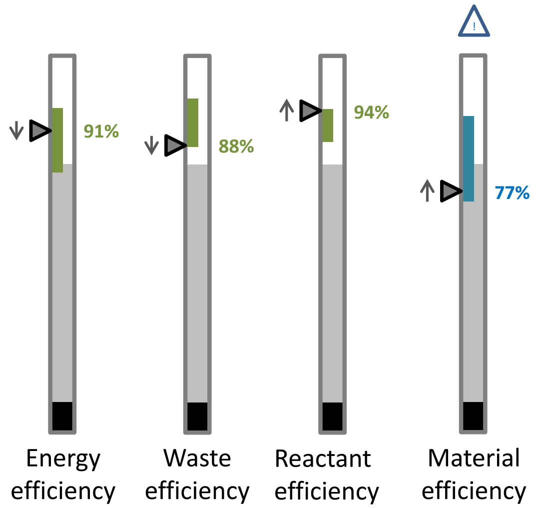


Figure 5.8: Bullet chart representation with current value, direction of movement, historical variability and relation to target value.

a minimization task) or with an orientation from left to right, depending on the available dashboard space and the given context.

Stacked Bars and Stacked Area Plots

Stacked bars and stacked area plots are used to represent data that is meaningful when aggregated, for example, multiple types of consumed energy per product that add up to the total energy consumption. The distinction between stacked area and stacked bar plots is made, because the same data is perceived differently (cf. figures 5.9 and 5.10). In area plots, the integrals of the contributing factors are naturally recognized and compared against each other. Furthermore, it is easier to compare more distant states in time by simply imagining a horizontal line in the diagram, i.e. the steam consumption in October 2012 rises above the initial value at the end of 2011 after a low value in April 2012. It is also visible that the electricity and steam consumption are exchangeable, because of the fact that the change in the overall energy consumption is small. Stacked bars on the other hand are perceived as units at each instance, which naturally implies their use for batch processes. For continuous processes, bars are sensible for fixed reporting intervals. Owing to perceptual effects it is easier to compare bars in close time proximity, because they are associated with specific points in time (cf. fig. 5.10).

Difference charts and sparklines

Line plots are a common tool to visualize data and help identify trends in time-dependent data sets. However, the utilization of line plots in the decision-making process for operational decisions, requires the users to consider additional information. By including information about equipment limits, process knowledge and experience, unnecessary cognitive effort is avoided. Alternative designs for sparklines are presented in figure 5.11. If

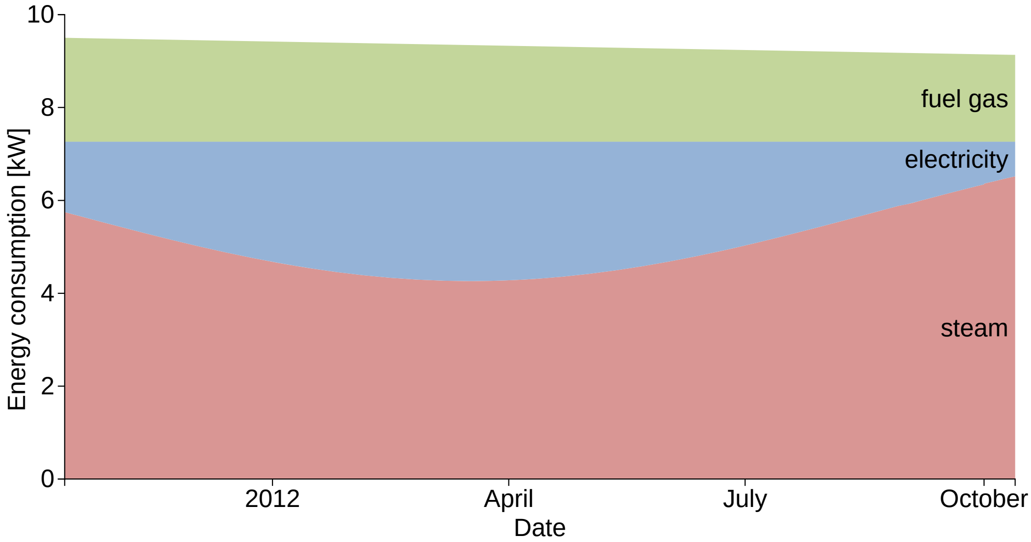


Figure 5.9: Stacked area plot.

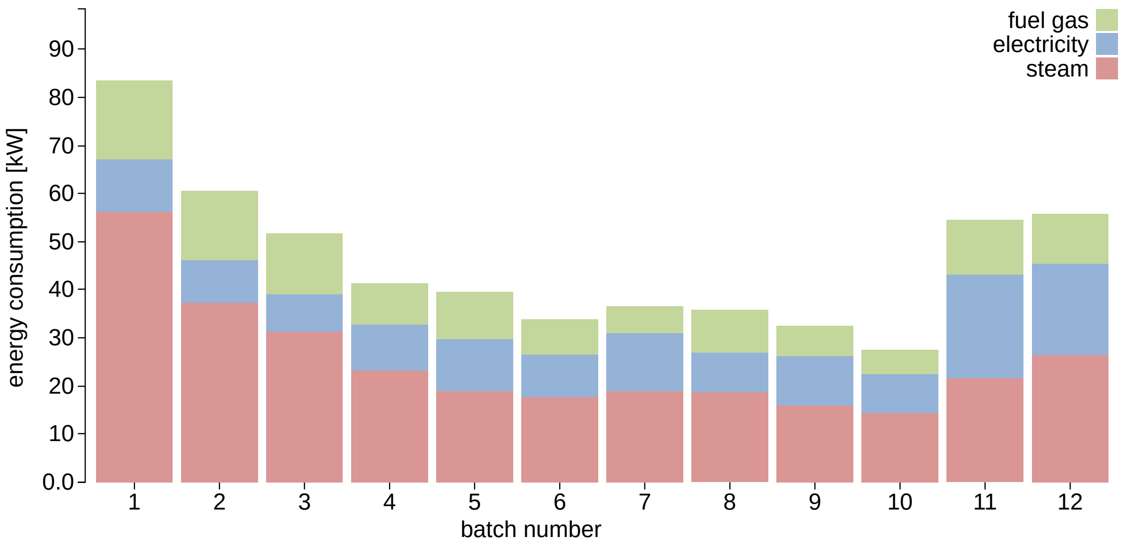


Figure 5.10: Stacked bar chart for batch applications.

only the indicator trend in relation to the current value is important, the sparkline is used with a minimal amount of dashboard space and distracting non-data pixels (Tufte, 2006) (top). If meaningful targets or bounds are available for the indicator, they can be displayed additionally to reveal violations and exceptions to the target levels (see bottom of fig. 5.11).

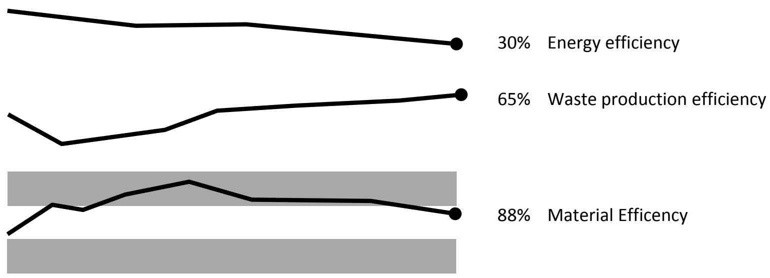


Figure 5.11: Sparklines for three REI in different setups.

Difference charts (cf. Figure 5.12) are another realization of line plots and are well suited to depict REIs in reference to a target value. By color coding the areas enclosed between the reference and the measured data, the saved amount is depicted as dark and the lost amount by light shading. With this visual aid it is possible to compare the resulting areas and to evaluate the operational performance. If the conditions are changing, owing to a different production volume or external influences, the reference changes, as seen in Figure 5.12. If there is reason to expect a large number of changes in the reference, the ordinate should be changed from absolute values to a positive and a negative deviation in percentages from the reference. Thus, the reference appears as a straight line on the abscissa, resulting in improved perceptibility.

Aggregated Tiles

The data representation with aggregated tiles (cf. Figure 5.13) uses color coding in order to show a certain property of a data set. In this instance, averaged REIs over intervals of 30 min are depicted as square tiles that can be evaluated by matching the color to the scale below. For an inefficient state of the indicator, dark shades are used, in contrast to efficient operating points that are represented with brighter shades. The arrows on the right supplement the historic development and denote the current state by color and the direction of movement in the orientation of the arrow. This visualization method does not provide detailed quantitative information, but helps in the comparison of indicators that cannot be directly translated into each other because of the use of different units or due to the fact that they monitor different effects. It is even possible to compare batch process data with data of a continuous process alternative, if required. The user intuitively recognizes trends in the respective row of each indicator and can furthermore identify pairs

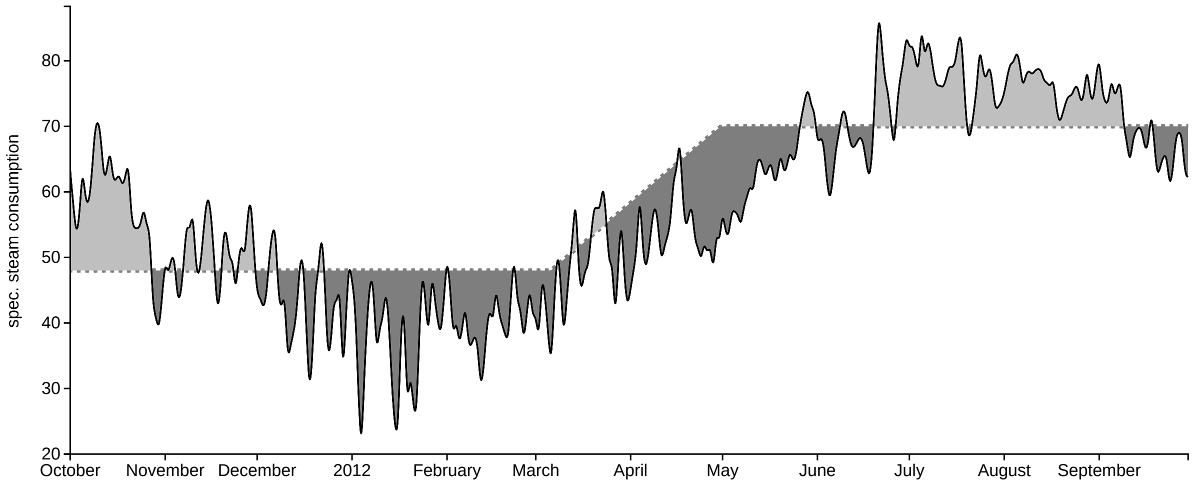


Figure 5.12: Difference chart to reference: light areas are losses compared to reference, and dark areas are gains compared to reference.

or groups of indicators that are correlated. The aggregation interval needs to be chosen carefully for continuous data, in order to be meaningful. In case the data origin is a batch process, each tile should represent a batch or campaign.

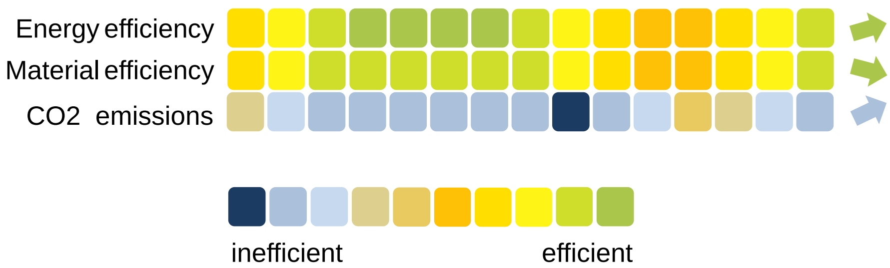


Figure 5.13: Aggregated tile plot with colour according to the efficiency.

5.2.3 Selection of visualization elements for efficient concepts

In the previous section, eight data visualization elements were evaluated for their suitability to represent REIs in context-dependent monitoring applications. A comprehensive overview is given in Table 5.1. If the considered method fully meets one of the requirements listed on the left, then this is indicated by a "+" sign in the corresponding field of the matrix. An "○" sign is used if the criterion is partially met and the field is left blank if the form of presentation is not suitable for the requirement. If the selection criteria for a planned visualization task have been defined, Table 5.1 can help select appropriate methods to create the most efficient dashboard solution.

The monitoring of resource efficiency in chemical production plants is a complex multidimensional task that requires highly efficient human-machine interfaces to convey informa-

Table 5.1: Comprehensive overview of the visualization methods introduced.

		Visualization element							
		Plant structure diagram	Sankey diagram	Aggregated tiles	Bullet charts	Stacked bars	Stacked area plots	Sparklines	Difference charts
Properties	Plant overview	+	+	○					
	Qualitative	○	+	+				+	+
	Quantitative		+		+	+	+		○
	Batch data		+	+	+	+			
	Continuous process data		+	○	+	○	+	+	+
	Trends		○	○	+	+	+	+	
	Many indicators (> 5)		○	+	+			+	
	Indicator history			○	○	+	+	○	○
	Fluctuating data				+	+		+	+
	Absolute	+	+	+	+	+	+		+
	Relative	+		+	+	+	+		+

tion on the process state to the operators. Since the amount of information that can be comprehended is limited, the focus of the operator needs to be guided towards the most relevant information at any time. An effective visualization uses the simplest and best suited method to relay information about an aspect of the data. In most cases, it is not possible to display all aspects equally well in just one diagram; thus it is beneficial to use complementary methods that highlight different aspects, i.e. a plant structure diagram with bar indicators for the total efficiency of the section can be used to show the overall state, along with stacked bar charts that further break down the contributing factors of the overall efficiency. With a smart selection of visualization techniques that highlight important data, very efficient human machine interface (HMI) can be created.

5.3 Design of a decision support system (DSS)

In the operation of production facilities in the process industry, the operating teams have certain degrees of freedom, which can be used to optimize the throughput or yield of the plant. Decision support systems for resource efficiency optimization should consider REIs and economic measures to choose operational parameters. As outlined before, the resource efficiency is described by a multidimensional set of indicators, where the Pareto-optimal operating regimes are described by the points on the Pareto frontier. The tasks of the system can be summarized as follows:

- depiction of the Pareto-front that comprises the set of Pareto-optimal operating points with respect to the REI and economic benefit,
- accepting input to obtain the user preference with respect to the resource efficiency performance,
- navigation on the Pareto-front,
- visualization of information to understand trade-offs,
- generation of understanding how the selected Pareto-optimal operating point can be achieved.

The human-machine-interface (HMI) is at the center of the DSS solution and must function in the most efficient way to minimize errors and avoid a cumbersome user experience. Guided by the classical design strategies (see section 5.1) the design process centers around the environment in which the system is used, the goal that should be reached, what the most likely steps in the thought process are, and how the information can be conveyed to the user with minimal loss of information using tailored visualization elements (see section 5.2).

Below, the key steps in the design of decision support systems for resource efficiency optimization are outlined, which work towards solving the tasks stated above:

1. Decide upon the scope of the decision making process, e.g. if it includes knowledge of the Pareto frontier or if the support entirely relies on current and historical indicator values.

2. Divide the decision making process into logical steps, that build on each other.

3. Identify the user group that has influence on the resource efficiency and analyze the users' experiences and system knowledge. Subsequently, the work environment is characterized to identify possibilities and limitations.

4. Based on the working environment, the users degrees of freedom and decision making process, choose the most efficient visualization elements to deliver the information

necessary for each step. The conceptual design selects the right visualization elements to efficiently present the relevant information and arranges them according to the logical sequence of considerations.

5. The design should be evaluated and discussed by domain experts to find flaws that hinder efficient interpretation and generate ideas for improvements.

6. Depending on the required maturity of the solution user acceptance tests or usability analyses can be performed to further improve the quality.

All considerations within the design process aim to make it easier to interpret the information to come to the optimal conclusion for the given decision problem. The concept of resource efficiency indicators are the basis, since they summarize the relation between resource inputs to the obtained products. An efficient dashboard design ensures that the information is displayed unambiguously, keeping errors during the interpretation process at a minimum. Furthermore, users are more likely to use the system if the effort for it's usage is low.

5.3.1 User environment analysis

The success of a decision support system crucially depends on the efficient cooperation of the user with the system. For this, it is essential to adapt the system to the user's level of knowledge about the production process and the relationship between the process parameters and their effects on the resource efficiency of the process. If too much basic information is provided, which can be presupposed by an experienced user, the interface will be unnecessarily overloaded. In this case, the user has to search for the relevant information or situations occur in which irrelevant information is mistakenly used for evaluation. On the other hand, inexperienced users may fail to recognize correlations between operating parameters, system behavior, and efficiency due to lack of experience. The risk of overloading can be minimized by a good knowledge of the user pool. With respect to inexperienced users, supporting information can be implicitly represented by graphical elements (e.g., system boundaries) or made available in the form of tool tips only when requested.

In general, the form of presentation should follow the type of information presented (see section 5.2.2), but the decision should take into account which forms of presentation are already known to the user community through training and professional experience. In this way, it is possible to reduce the time of familiarization and errors during the use.

Another factor in the analysis is the presentation medium. It is crucial to know which digital devices are chosen to display the decision support system. If an application on mobile devices by personnel in the plant is planned, the interface must be designed for operation on smaller screen sizes and with touch functionality. If use in the control room or an office environment for plant management or technical support is envisaged, the available screen size is larger and input is done via mouse and keyboard.

5.3.2 Decision analysis

The decision making process during the optimization of resource efficiency in the process industry consists of the steps shown in fig. 5.14.

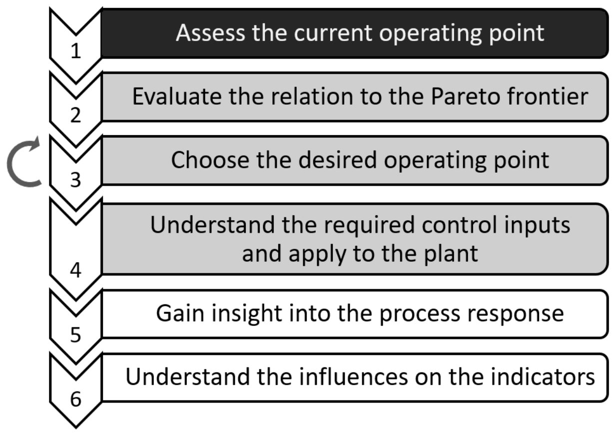


Figure 5.14: Steps in the decision making process for the resource efficiency optimization of a chemical production process. The background colors correspond to the level of decision support.

In the first step, the current operating point is evaluated using the REIs. In order to do so, the indicator values must be provided separately and in relation to a reference value. The reference value can be a historically observed performance or theoretical optima. If the Pareto frontier is available the relation of the previous operating point to the Pareto frontier is assessed to obtain the improvement potential (step 2). In case of sub-optimality, the distance of the closest operating point on the frontier in the direction of each indicator is of interest, since each signifies how much optimization potential is available without the need to deteriorate another indicator (see section 4.1.1 on Pareto optimality). Afterwards, the user needs to choose the performance for the next batch (step 3), ideally on the Pareto frontier. In the simplest case, this means to optimize the most important indicator according to the preferences of the user. If other motivations are present, e.g. a minimal constraint on any of the indicators the user needs to navigate on the frontier, while being subject to the physical process constraints. This process might need some iterations to evaluate alternatives to achieve this goal. The forth step is to evaluate the input variables that are predicted to achieve the desired performance, to apply them to the process and to potentially revisit the DSS, e.g. at times of changing external motivations. The remaining steps aim to increase the process knowledge and influences on the performance. The process of insight is twofold, first the inner relation or cause-and-effect relationship between the inputs and the process variables need to be understood (step 5). The second part means to see how the relevant variables influence the indicator values and hence in the trade-offs between them.

It is not necessary to go through all steps to realize decision support. The process can be logically divided into three levels that are indicated by different background colors in fig. 5.14. They are subsequent and built on each other. The first level is made up by step 1, where the current operating is evaluated. This is the most simplistic assessment that can be used to optimize the process parameter by trial and error. The second level includes the steps 2 – 4 and requires a process model to obtain the Pareto front. The creation of a model and the execution of an optimization are associated with an increased effort. However, this additional effort makes it possible to select an optimal operating point. Furthermore, the Pareto front provides a description of the trade-offs between the indicators and their minima and maxima. The associated process parameters can then be adopted by the user to optimize the process. The third level additionally includes steps 5 and 6 which are not necessary for an optimal operation, but can contribute to the confidence in the system.

5.3.3 Conceptual design

As outlined in the previous section 5.3.2, the DSS is intended to (goal 1) prepare information to enable the user to make operational decisions including the required inputs, (goal 2) to explain the trade-offs between the indicators and (goal 3) to understand the inner process relations. The third goal is optional, but useful to create trust in the DSS at the beginning of the DSS life-cycle. A reduction of the cognitive effort is necessary in the context of multi-objective optimization, because it is hard to understand the problem in its full complexity. Furthermore, tasks with a higher cognitive load are more error prone. The skills-rules-knowledge (SRK) framework developed by Rasmussen (1983) models the decision making on three distinct levels that vary with respect to cognitive load (see section 5.1.1). The ecological interface design (EID), described in section 5.1.2, builds on the SRK framework to develop interfaces that show preprocessed information to reduce the necessary reasoning process for the user.

According to the SRK framework the most cognitive effort is used in the knowledge-based reasoning that requires the interpretation of complex information and possibly process experience of the system under investigation. This is the case for multi-objective optimization tasks, since the operational degrees of freedom during batch production are dynamically affecting the concentrations and temperature. This will subsequently affect the product and waste formation and finally the resource efficiency performance and profit. To achieve goal 3, the user must perform considerations on the knowledge-based level. Facts and experience must be considered and referenced against the indications made by the REI. Here, the goal must be to reduce the cognitive effort for the perception of the information to a minimum, by displaying it in an intuitive and accessible way. This reduces the necessary abstraction steps and hence the cognitive effort for interpretation.

A central challenge is the representation of the Pareto front and the resulting relationships between the competing REIs that describe the resource efficiency. Typically the optimization problem is three- or four-dimensional, which can be represented in a coordinate system with color coding one of the indicators in the four-dimensional case. However, a correct interpretation of such a representation is complex and hence error-prone. Section 5.2.2 proposes multiple visualization elements that can be used to indicate REIs. A good option are bullet charts that are similar to parallel coordinate plots and can display a high number of indicators if needed. The selection of one indicator will limit the available range on the others. Thus, the user can experience the trade-offs similar to a What-If analysis by manipulating the indicators and observing the the effect on the others. To be able to observe the relationships between all indicators, they all have to be displayed simultaneously and clearly arranged. Thus, the user does not have to keep performance figures in mind but can compare them directly, which minimizes the cognitive effort for the objectives (1) and (2). In order to fulfill the optional objective (3) a similar approach is pursued by visualizing the differences of inputs, system dynamics and the resulting performance measures for the current selection in relation to the reference point. As soon as trust towards the decision support is gained, the user is confident that the REI capture and indicate the efficiency correctly. At this point, decisions are made solely based on the indicator values and resulting trade-offs by accepting the DSS suggestion without reconstructing the inner process dependencies. Thus, the interface usage is reduced to the rule-based interaction during a What-If analysis and selection procedure. This reduces the cognitive effort according to Rasmussen (1983) and will decrease the error rate.

The last two steps of the decision making process, outlined in fig. 5.14, are optional and will only be used during the instructional phase of its use. Hence, the structure of the dashboard should be arranged to prioritize the visualization elements necessary for the first four steps of the decision making process. As outlined in fig. 5.2, the general reading direction for western users is left to right and top to bottom. Thus, the indicator overview and interaction panel must be placed in the top left corner. Depending on the necessary size of the other required visualization elements, they should be arranged to the right or below for a natural flow of usage (see fig. 5.15). The four areas of the DSS contain:

Overview: A part of the interface must be dedicated to explaining the current values for the REIs in relation to the benefit situation. Ideally, the visualization element also

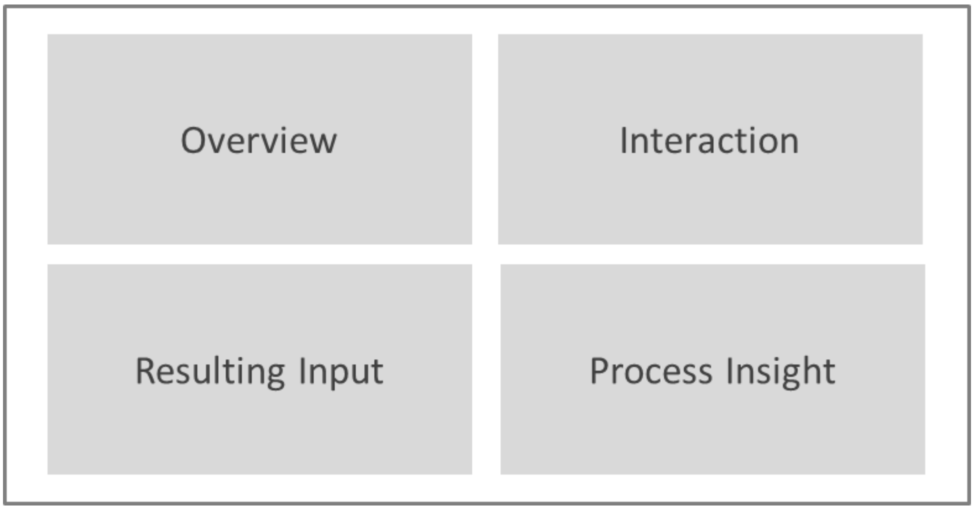


Figure 5.15: General interface set-up, following the design rules in section 5.2.

includes the optimization potential available.

Interaction: The second functional area of the interface must be a panel that allows for intuitive interaction to select the desired position on the Pareto frontier, in terms of the indicators. Ideally, the manipulation directly invokes an update of the remaining visualization elements that correspond to the newly selected Pareto point. If possible, the interactive elements can be integrated into the overview panel.

Result: The third part should explain what process inputs are needed to achieve the desired performance. The user can either accept the solution and apply it to the next batch instance or advance to the next visualization element.

Performance insight: The fourth element of the interface is dedicated to create trust into the underlying model and methodology. This element will depict the causal chain from the process inputs to the predicted performance outcome.

At the end of the process, the design should be evaluated by domain experts. For the expert interviews, it is not mandatory to fully implement the dashboard; mock-ups of the individual elements are sufficient. It makes sense to evaluate the functional parts of the dashboard separately; the sections in Figure 5.15 are suitable for this purpose. For each section, the domain expert should first be asked, how he or she would implement the display without having seen the design draft beforehand. In this way, new ideas can be generated uninfluenced, in case a change to the design becomes necessary. The experts then give their assessment of the proposal. At the end of the interview, the overall composition is evaluated by simulating the entire decision-making process. The collected results can be used to optimize the proposal.

5.3.4 Technical implementation

In addition to the conceptual preparation of the interface, it is important to achieve a good technical implementation. An interactive system for decision support requires not only the display of selected visualization elements but also a high-performance interaction in order to capture user input as easily as possible. As with the use of any software, the functionality of the interactive elements should be designed intuitively. This minimizes incorrect input and the resulting irritation of the user. Waiting times interrupt the workflow and should be avoided.

Consideration of the following tips will optimize the implementation of REI decision support systems in processing plants:

- If the dashboard contains secondary information that is only displayed upon user request, make sure that the presence of this information is apparent or pointed out to users.

- The operation of the interface should be implemented using common technological solutions and adapted to the environment in which it is used. For example, if the dashboard is to be used in the field, it must be optimized for user input on a mobile device via a touch interface.

- The device must have sufficient computing power and bandwidth to enable a smooth and uninterrupted experience.

- An implementation on digital platforms that are freely available within the organization is helpful to allow transferability to similar applications. These can be proprietary software solutions for which the company or potential customers hold appropriate licenses, e.g. Matlab or BI tools, or can be based on open-source technologies such as JavaScript, Plotly Dash or others.

- Computationally intensive operations should be avoided that can impact performance. By precomputing the optimization results, it the results only need to be filtered as requested by the user.

5.4 Application case: decision support for Williams-Otto semi-batch reactor

The goal of this work is to design a decision support tool for the optimization of resource efficiency for batch and semi-batch plants in the process industry. The framework for the definition, calculation and presentation of REIs in batch processes developed in Chapter 3, was applied to the Williams-Otto semi-batch reactor (WOSBR) benchmark process in section 4.2 and was solved as a multi-objective optimization problem using state-of-the-art optimization methods to obtain the Pareto front.

The result of the optimization is used in the following to create a decision support solution for the WOSBR with the help of which the user can select a Pareto-optimal operating point according to the efficiency targets. Since four efficiency indicators are relevant for the chosen example, the Pareto front represents the trade-offs between those four competing interests. The Decision Support Interface should display the inputs that will be leading to the desired operational point. Furthermore, the user should have all the necessary information to understand which relationships will lead to the desired outcome.

The intended tasks, stated above, guide the design process. The design framework developed in section 5.2 is applied to obtain the DSS solution. First, a detailed analysis of the decision making process is conducted below and based on the obtained information a tailored conceptional design is developed subsequently. In the end it is evaluated by interviews with domain experts that challenge the initial design. Based on the findings of the interviews, an improved alternative is derived that is implemented as fully functional interface. To assess the quality of the DSS an experimental trial was performed as described in Chapter 6 to see weather the DSS can be understood and effectively used by the participants of the study.

5.4.1 User environment and decision analysis

For the decision support in the considered process, a model was available and was used to derive the Pareto front. Therefore, it is possible to reach the highest level of decision support according to the scheme in fig. 5.14. The resource efficiency, in combination with the economic performance is represented by four indicators. The relationships between the indicators are complex and difficult to represent, since a representation in coordinate systems is limited to three dimensions and extended forms of representation such as coloring represent a high degree of abstraction. Thus, it is important to find a well understandable representation for decision support and to adapt it to the user environment and experience.

The WOSBR is a theoretical process, but it is comparable to industrial processes for specialty chemicals. Users of the system must be able to make decisions about the operating point. If the changes are minor, plant operators can make a decision to change setpoints within the degrees of freedom in the process operating procedure. However, in the case of the WOSBR, there is a significant impact on the profitability of the process, as indicated by the Benefit Indicator, and the decision is to be done by the management. This group of people work mainly in the office environment and have standard

PCs with keyboard and mouse input at their disposal. There is no time pressure in the decision, but a short processing time improves the user experience and work efficiency.

The first step of the decision process is to assess the current operation in relation to the maximum possible resource efficiency per indicator. The information needed for this are the values of all indicators, as well as the extreme values on the Pareto front. The indicators have different units and are therefore difficult to compare with each other in absolute terms. Helpful for the interpretation is to put them in relation to a reference, this can be the current or the maximum achievable indicator value. The assessment of the current performance is followed by the selection of a new Pareto-optimal operating point. The starting point for the selection here can be the previously assessed potential for improvement per indicator or a target set by the user, such as improving energy efficiency or optimizing the yield (material efficiency). If the previous operating point is suboptimal, the selection is trivial and a Pareto-optimal operating point, with equal efficiency on all other indicators, can be used. However, if the operating point is already Pareto optimal or if the optimization potential by moving to the Pareto front is not sufficient, an improvement can only be bought by a deterioration of another indicator. It is therefore useful to show the consequences of an optimization of one or more indicators. This can be achieved either by a graphical representation of the sensitivities or in a dynamic representation of the possible range of outcomes on the deteriorating indicators. The shape and position of the Pareto front determines whether a desired performance combination of indicators is possible and the user should be able to recognize this. Once an acceptable combination of performance indicators has been found, the corresponding input variables must be displayed. For the WOSBR these are the feed profile, as well as the heating and cooling power curve over the fixed batch length. After inspection the user is able to apply the suggested parameters to the plant.

Decision support for optimizing resource efficiency is not an established method in industrial practice, thus promoting the users' confidence in the method is necessary. For this purpose it is necessary to explain to the users why suggested changes on the parameters will result in the desired change in performance. This includes showing the evolution of inputs and the resulting dynamics of the reaction. This in turn causes the batch outcome, from which the indicators values are derived.

5.4.2 Conceptual design

Following the decision analysis, the plant management will be the primary target group for the decision support. This group has a profound technical background in chemical engineering. For the design of the interface, knowledge of the use case and the reaction system is assumed. The following five general requirements were identified to be most relevant according to the considerations in section 5.2.1:

- If complex considerations are necessary, a concise training should explain the necessary background information. This aims to minimize the learning phase until the tool can be used efficiently.

- Self-explanatory design, regarding the functionality.

- Efficient interaction is enabled by interactive elements that are easy to use and react as expected, with little interaction.

- Transparent cause-and-effect relationships explaining why a certain solution is optimal and how the proposed process inputs lead to the requested process performance.

- Maximum accuracy of the displayed information creates trust and acceptance thus, fostering the usage of the DSS.

Monitoring task: Taking the above requirements into account, the current efficiency for all four indicators must be presented first, as it is the starting point for the decision. The sole representation of the value is not meaningful, therefore the optimization potential is expressed in terms of the distance from the Pareto front in %. With respect to the front, each of the four potentials correspond to the projection of the last operating point onto the Pareto surface in the direction of the indicator. For each indicator the minimum and maximum of the corresponding indicator on the frontier are used for scaling. 0% corresponds to the worst value of the indicator and 100% to the optimum. According to the definition in equation 4.15, the indicator value is maximal at the optimum. The potentials are indicated by the difference to the optimum (100%), which must be less than zero and can also take values below the -100% points if the previously observed performance is worse than the minimum on the Pareto front. The indicated potentials cannot be achieved simultaneously. A table is chosen as the form of presentation, because the amount of information is small and the relative position to the Pareto front is sufficiently well captured by the scaling. Thus, the table shown in fig. 5.16 is the first visualization element of the DSS.

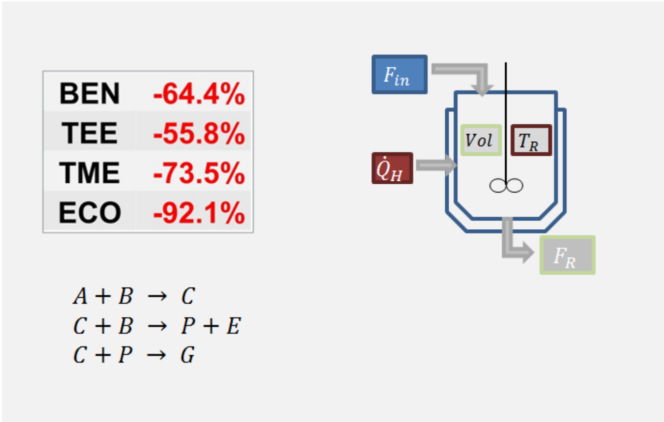


Figure 5.16: First dashboard draft for the monitoring section.

In addition to the efficiency of the preceding operation, the reaction system and the sequence of the semi-batch process are important to gain process understanding. Thus, a schematic representation of the reactor with the relevant process variables and the reaction equations that are involved are displayed (cf. 5.16).

Pareto navigation: After the user is informed about the possible optimization potentials, the selection of a new operating point from the set of Pareto-optimal points begins. To do this, the user must be able to interact with the dashboard to either vary the process inputs or to adjust the performance indicators. If the inputs are varied, the user must find the right combination of inputs through experience and understanding of the system to find a desired result. If the performance indicators are manipulated, the corresponding inputs are known from the optimization and can be displayed. E.g. three parallel and interdependent reactions take place in the WOSBR, which are influenced differently by the reactor temperature. The obtained amount of the components P and E is included in the calculation of all indicators. Thus, the feed profile of the reactant B as well as the imposed cooling or heating power has an indirect influence on the resource efficiency indicators via the reaction system. Such a complex system can only be optimized with an extremely high intellectual effort to arrive at a desired performance. Thus, the indicators are chosen as manipulated variables.

Since a representation within a coordinate system is only straightforward for two dimensions, as explained in section 5.2.2, bullet charts are recommended in the case of four indicators. These act like parallel coordinates and display the indicators as shown in fig. 5.17. The bullet charts are scaled to the range of the Pareto front (0%–100%) and the current indicator values are shown as triangles. The scale in [%] corresponds to the same scaling as above with respect to the minimum and maximum value of each indicator on the Pareto-front.

To bridge from the monitoring table to the navigation, the performance of the preceding operating point is also depicted in the bullet by green triangles (see fig. 5.17). Below each bullet chart, the user can manipulate the indicator using a “+“ and a “-“ button. The gray bar between the buttons indicates the possible range for the indicator, which is coincident with the Pareto frontier position in relation to the current point. Figure 5.17 shows the initial state with roughly 99% for the benefit indicator BEN, thus the possible improvement is small, while the range for deterioration is 99% as indicated by the gray bar. A similar picture emerges for the total material efficiency TME. The other indicators are currently at 50% and 0% for the TEE and ECO indicator, respectively.

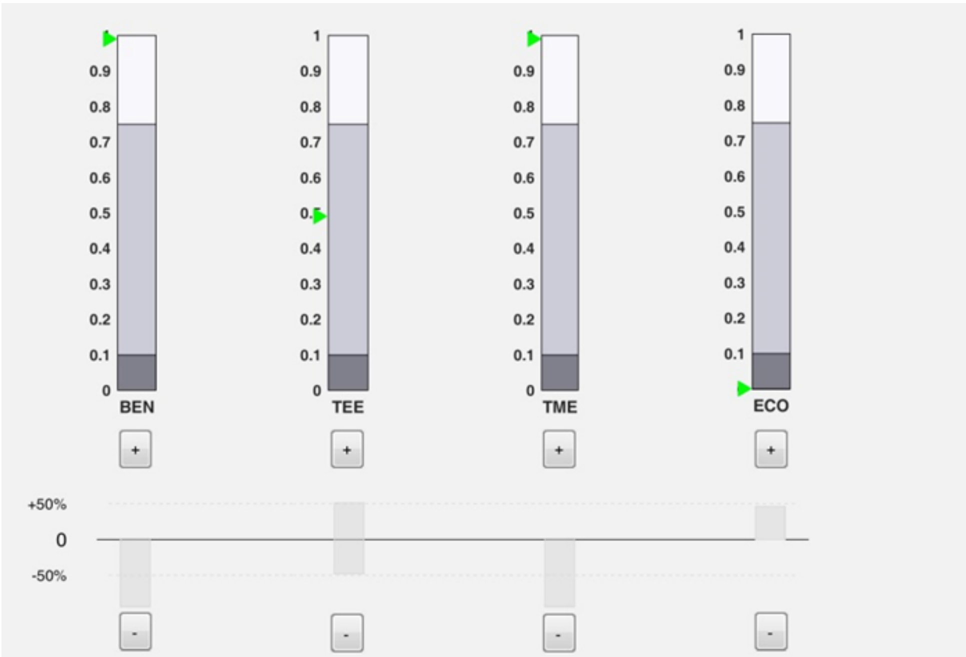


Figure 5.17: Bullet chart representation of the REIs for the WOSBR application case (top). Below the selection tool indicates possible ranges and enables the user to interact by buttons.

Upon interaction via the plus and minus buttons a new operating point can be selected (see fig. 5.18). Using a simple click increases or decreases the indicator by 1%. If it is held down, the tool will perform a step of 10% every second to cover larger ranges fast. As soon as there is interaction on one of the indicators, the other indicators can only assume a smaller subset of values, since not every combination of indicators is possible. Thus, the gray bars in the lower part of the interface are dynamically adjusted to show the remaining ranges for the remaining degrees of freedom. This can be seen in fig. 5.18 for TEE with the current selection of +25%. The benefit was previously selected to be reduced by −5%. The remaining ranges for TME and ECO are small for the current selection of TEE.

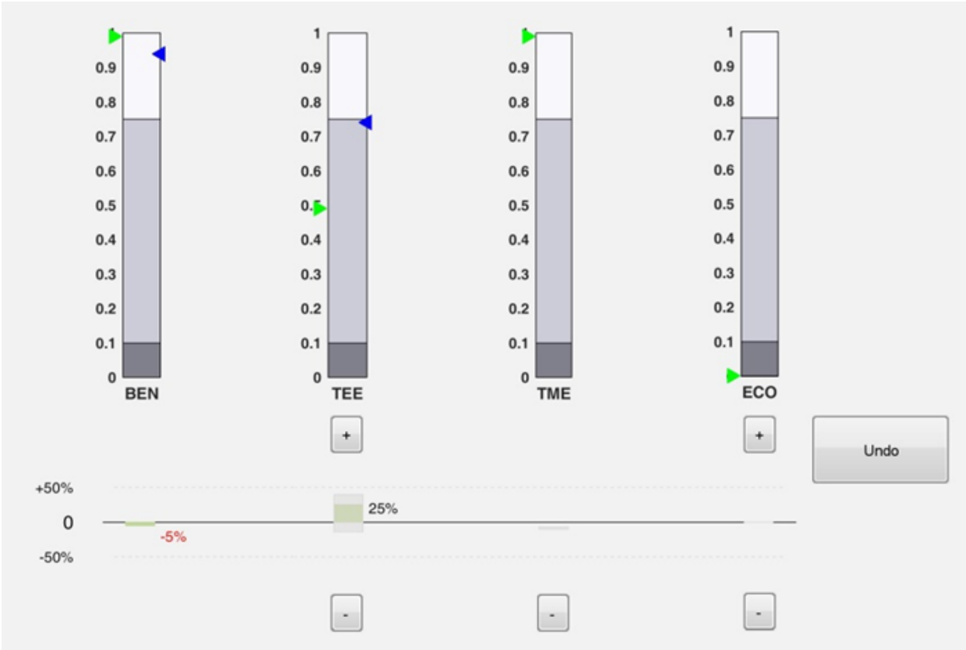


Figure 5.18: State of the performance selection tool after the user already selected the economic performance (BEN) and is currently choosing the desired performance for energy efficiency (TEE). Green triangles indicate the previous operating point, blue triangles indicate the selected performance for indicators that were already manipulated in the selection process.

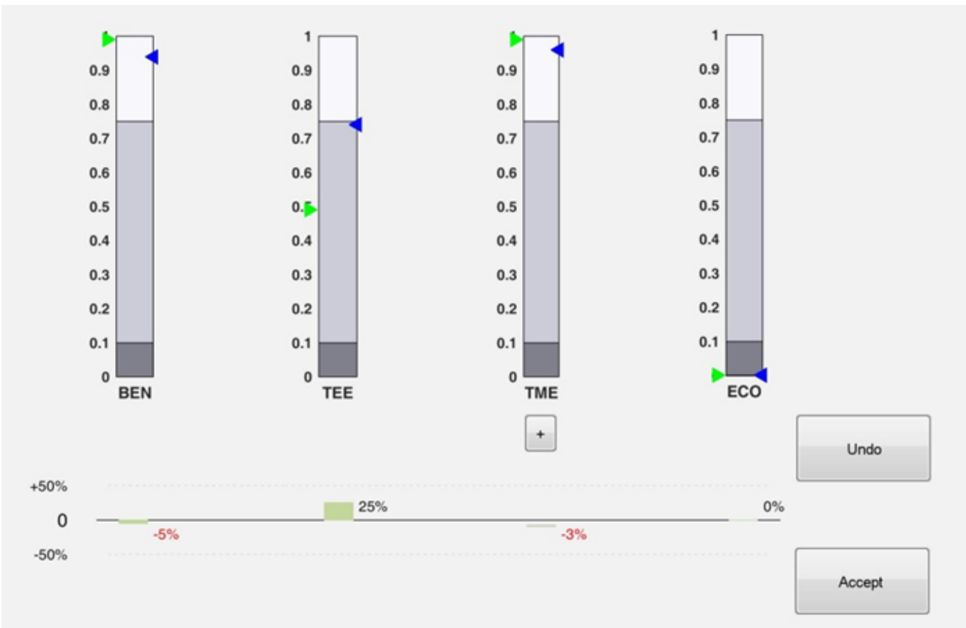
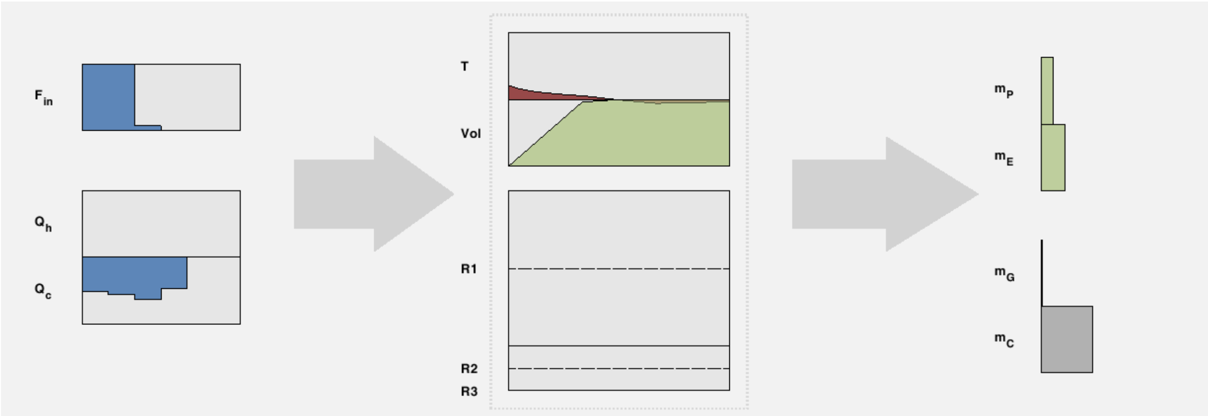


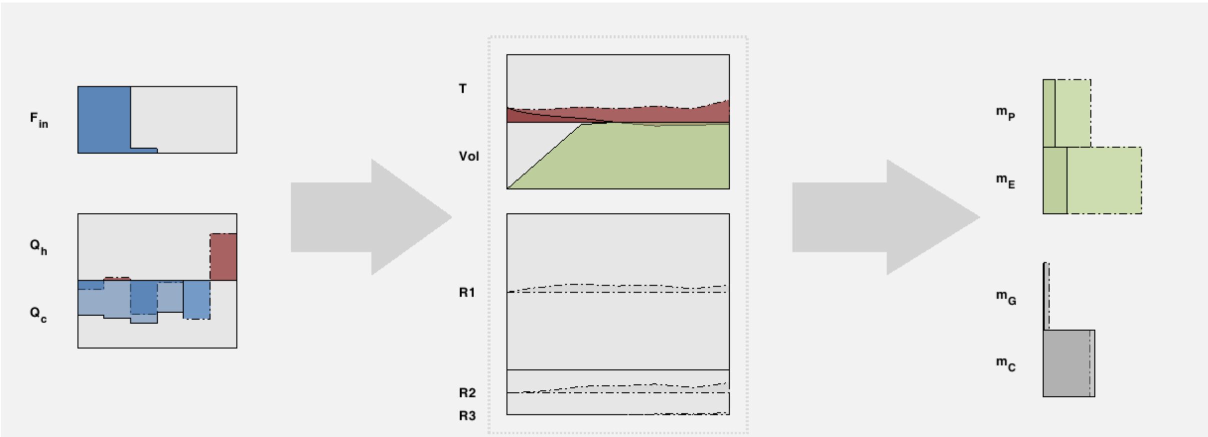
Figure 5.19: Final state of the performance selection tool after the user selected a new operating point.

Having already chosen the desired value for benefit BEN and currently manipulating the total energy efficiency indicator TEE as shown in fig. 5.18, the buttons for BEN are disabled. Furthermore, the "+" button for the total material efficiency is disabled, because the remaining range for it is completely below the previous operational point. The decision process is continued analogously until a specific operating point is selected. Right next to the decision panel three control buttons are located that can be used to revert the last decision or accept the selected point as final (cf. fig. 5.19). The differences between the previous operating point and the final selection are displayed in absolute terms in the bullet charts using the triangular depiction and relative to the initial point in the decision tool at the bottom with a percentage of change. The bullet charts in combination with the decision tool allows for efficient communication of the interrelations between all indicators. The user is enabled to chose the desired metrics balancing the contradicting interests. In case the desired combination of indicators is not possible, for example good ECO efficiency paired with a good total material efficiency TME, the user can observe that only low values for TME are possible as soon as the a good target value for ECO is selected. Thus, the user selects a preferred operating point on the Pareto front by sequential selection of the indicators. The previous selections can be reversed at any time using the "Undo"-Button and an iterative exploration is possible until an acceptable operating point is found.

Process insight: The dashboard area dedicated to insight generation shows the evolution of the previous operating point during the selection process. Manipulation of the third indicator also determines the value of the fourth as a result of the concept of Pareto optimality. As soon as the manipulation of the third indicator has started a unique point can be inferred from the user input and the part of the dashboard that is dedicated to insight generation is automatically updated. The causal chain of influences and effects has three elements: the evolution of process inputs, the reaction of the system to the inputs, and the final outcome at the final time t_f that determines the values of the efficiency indicators. Hence, the three steps guide the setup for involved visualization elements, c.f. fig. 5.20a. The evolution of the inputs and of the response of the system over time are displayed using graphs with two axes. The graph on the upper-left shows the feed profile for material B, and below the heating or cooling profile is shown. The central element shows the progression of the reactor temperature in red and the volume of the reactor content in green. The evolution of the temperature is a result of the relatively cold input of B, the heating or cooling duty, and the reaction enthalpy of all reactions. Since the operation mode is semi-batch, the reactor volume is only affected by the input stream of B. The horizontal axis in the diagrams at the left and center starts at time zero and terminates at the fixed final time t_f. The upper and lower constraints on the feed profile, the heating and cooling trajectories, the temperature, and the reactor volume are shown by the boxes around the graphs.



(a) Initial detail view for the current input selection.



(b) Detail view with the current and possible next operating point.

Figure 5.20: Detail view of HMI alternative one with input (left) and output (right) visualization to compare Pareto-optimal operating points. The central element explains the evolution of the variables of the batch and the relationships between them.

The lower three boxes in the middle are associated with the instantaneous reaction rates calculated according to equations 4.8a–4.8c. The absolute height of the box is fixed and it is vertically divided into three areas for the three reaction rates. The sizes of the areas depend on the ratio between the average reaction rates at the previous operating point. Here, reaction rate R1 is the largest and R3 close to zero. Each vertical axis shows the difference between the reaction rate trajectory of the previous batch and the selected point. Without a selection the graphs are blank, because no difference can be calculated.

The outcome of the batch in terms of the product yield is shown for the reaction products P, E, G, and C on the right hand side, by horizontal bars. Since the outcome represents only one point in time, only one dimension must be shown. The bar width depends on the amount of each component at the end of the batch in $[kg]$, with shared y-axis to make the amounts comparable.

By iterative testing, the user investigates how the changes made to the operation, shown on the left, impact the progression of the batch, in the center, and subsequently the outcome on the right hand side. In order to reverse a selection, the user can click on the "Undo" or "'Reset" button as shown previously in figs. 5.18 and 5.19. Until the user selects a specific operating point (less than three indicators, c.f. fig. 5.18), the part of the dashboard dedicated to process insight only shows information associated with the previous operating point (cf. fig. 5.20a). The new operating point will show up as soon a new point is selected and is shown by dashed lines (c.f. fig. 5.20b), whereas the previous one is depicted using solid lines. For the example shown, the overall cooling duty is reduced and during the last time interval the batch is even heated. This results in a higher temperature level and increased reaction rates, as can be seen in the central element. This in turn increases the amount of products P and E significantly, while the absolute increase of the toxic side product G and the intermediate compound C is small. Based on the visualization, the user can comprehend how the selected Pareto optimal solution can be achieved. Here, the increased amount of product is achieved based on the same amount of raw materials. This leads to a significantly improved material efficiency TME as well as benefit indicator BEN.

Initial design: The first design is shown in fig. 5.21 and it follows the composition rule in fig. 5.15 with the reading direction from left to right and top to bottom, where the panels dedicated to the resulting input and process insight are merged due to their close interconnection in this case.

The decision making process will start at the **top-left**, where general process information in the form of an indicator table, a schematic of the reactor, and the reaction equations 4.4–4.6 are shown. The table contains information on how much the current operational point can be improved for every indicator, where negative values indicate sub-optimal operation. The indicators are scaled to the maximum and minimum value for each indicator on the Pareto front. It is not possible to achieve positive values, but values of less than -100% are possible in case of a poor performance. The reaction and reactor schematic are shown to give supporting information to achieve contextual awareness. The WOSBR is depicted with the measurements: reactor volume Vol and temperature T_R, as well as the inputs: heat transfer $\dot{Q}_H$ and feed of B F_{in}. The output stream F_R indicates the final reaction mixture at final time t_f. The composition is relevant for the calculation of the resource efficiency indicators.

The user interacts with the dashboard in the **top-right** element. Each indicator is visualized with the help of a bullet chart (see section 5.2.2) that shows the currently selected operating point. Buttons are available to interact with the interface to perform the selection process. Fig. 5.21 shows the state after the selection process.

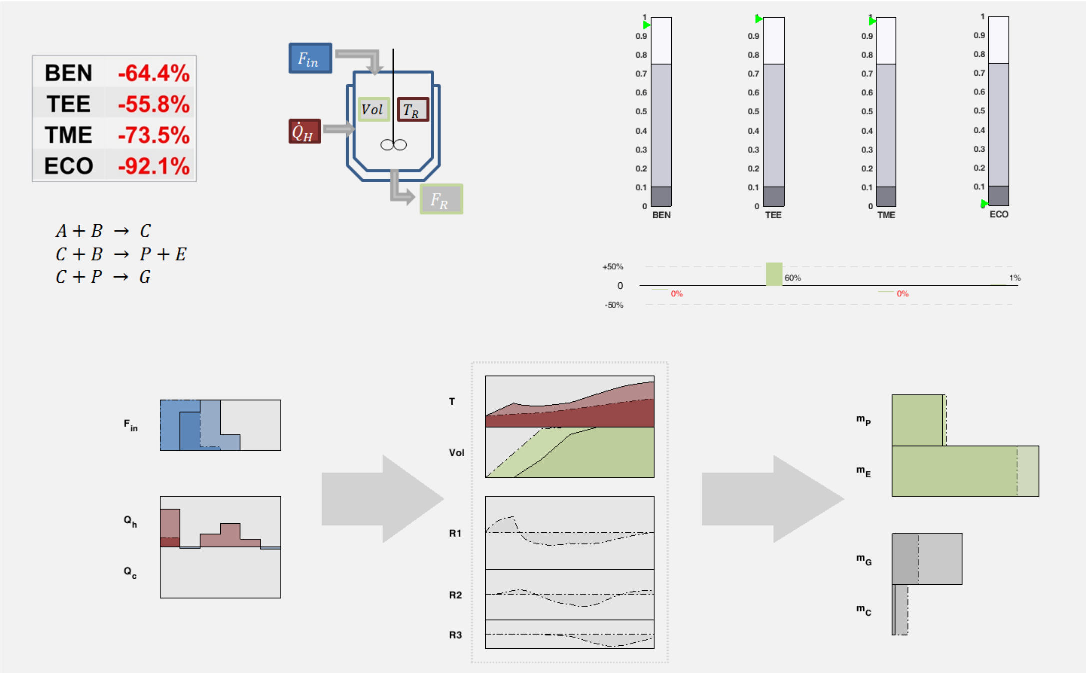


Figure 5.21: First version of the human-machine-interface for the WOSBR application case.

The **bottom** part of the interface is designed with the goal to explain the inner relationships of the process. Starting on the left, the input trajectories for the last batch and the predictions are shown. The relatively cold feed and the heat transfer profile result in the shown trajectories of the state variables of the model. The right part is dedicated to the amounts of critical variables obtained regarding the main influencing factors to the resource efficiency of the batch. With this information the user can comprehend how the changes lead to the new performance.

5.4.3 Expert interviews

Expert interviews were conducted with five experts form the Department of Biochemical and Chemical Engineering at TU Dortmund University that have a high level of expertise in the field of computer science, process dynamics, and control. The demographics related to the participants is summarized in tab. C.2 of the appendix C. The intention of the expert interviews was to challenge the initial design concept and to generate an improved concept, if necessary.

Each interview was performed according to the guidelines of a structured interview and was recorded in an interview protocol. The structure was chosen as:

(1) Introduction

  (1a) Definition and scaling of REIs

  (1b) Concept of Pareto optimality

  (1c) Introduction to the WOSBR process

  (1d) Resulting Pareto frontier

  (1e) Goals of the decision support interface

(2) Evaluation of the dashboard with independent idea generation and criticism of the visualization elements for each step of the decision support

  (2a) Monitoring task

  (2b) Pareto navigation

  (2c) Process insight generation

(3) Evaluation of the dashboard composition

First, the concept of resource efficiency indicators was introduced and deepened using a paper-based example (1a). The indicator definition followed the methodology in chapter 3 and was exemplified using a simple reaction system that showed the necessity for indicator scaling to the best and worst values on the Pareto frontier.

In part (1b) the concept of Pareto optimality was explained using a two-dimensional example with TEE and TME, based on the one given in figure 4.1. Next, the WOSBR process was explained and how the operational degrees of freedom affect the defined REIs (1c). Based on the theoretical considerations before, the solution of the arising multi-dimensional optimization problem was covered. The central result is the structure of the Pareto frontier created by consideration of the resource efficiency indicators: benefit (BEN), total energy efficiency (TEE), total material efficiency (TME), and the ecological performance measure ECO (compare fig. 4.7d). The introduction concluded with the functional targets of the interface:

- Relate the current operation to the Pareto frontier,
- navigate on the Pareto frontier and
- improve process understanding.

In the second part of the interview, the experts were interviewed regarding the three tasks (2a-2c). For each task, they were asked to list the required information and to create a first draft of a visualization element without being previously exposed to the design. The exploratory character of this task is important to enable the generation of new ideas, without being guided by predefined visualization elements. Each element was discussed regarding the points:

- Visual appearance and comprehensibility
- Case-specific functional alternatives
- Expected workflow
- Collection of ideas for alternative designs.

At the end of each interview (3), the proposed composition and logical structure of the DSS was discussed (cf. 5.21): top left for referencing the current operation, top right for navigation on the Pareto frontier, and bottom towards process understanding and decision support. The focus was on the questions:

- Is the composition suitable?
- Is there any missing information on the interface?
- Is it sensible to integrate elements towards monitoring, navigation, and process understanding in one dashboard?
- Are there any general remarks?

The following paragraphs summarize the results of the expert interviews. The summary does not contain all the feedback, but presents the most important aspects in the author's opinion. The complete interview transcripts are available in digitized form on the enclosed DVD.

Monitoring task: Based on the discussion with the experts, the following findings were compiled regarding the dashboard elements that are involved in the monitoring task. The table should be removed, since the monitoring information is also included in the bullet charts and thus redundant. With respect to the readability it was suggested to increase the font size and the size of the triangles. Since the position of the triangle is only giving an estimate of the exact value, an additional label next to the triangle, stating the indicator value as text, would improve the situation. The next topic of discussion was the relative position to the frontier. While the relative offset to the individual indicator extreme points on the frontier is constantly shown as difference to 100% and 0% on each chart, there is no indication on how easy or difficult it is to achieve operation in every part of the Pareto-front. An expert suggested to derive a measure that represents the available degrees of freedom on the other indicators if one is fixed. This is especially useful for cases where good performance on one indicator is not compatible with the others. For the WOSBR this is the case for the ECO performance indicator (see fig. 4.7d). It is suggested to color the bullet charts accordingly, to show that for good values on the ECO indicator there are only small degrees of freedom on TME, BEN, and TEE. An alternative approach to the coloring of the bullet charts is to base the coloring on the sensitivities, i.e. the mean derivative of the REI.

The experts pointed out that the reactor diagram and the reaction equations clutter the dashboard with to much information and coloring. A black-and-white representation of the reactor with clear indication of the manipulated process parameters, as well as the measured process variables temperature and level, is sufficient. The reaction equations were classified as secondary information, which should only be displayed on request by the user. Furthermore, the indicator definition must also be available as secondary information in order to understand how it is calculated. This ensures that the dashboard remains concise and the secondary information is still available.

Pareto navigation: Evaluating the draft of the navigation tool shown in fig. 5.17, 5.18 and 5.19, that consists of the bullet charts and the decision tool below, the readability was one focus of the discussion. To improve the dashboard the font size should be increased and it was requested to place the indicator labels at the top of each bullet chart to allow for a natural reading direction from top to bottom. Furthermore, the numeric values should be added next to the triangles and the scale is to be changed from decimal values to percent. During the inspection of the design concept, the majority of experts agreed to favor bullet charts over the alternative of 2D or 3D plots, due to a simple interpretation and scalability towards the fourth dimension.

There seem to be two plausible methods to manipulate the bullet charts. An integrated slider option was listed as an alternative to the interaction using buttons. If a slider is integrated into the bullet chart as an input element, the precision of selection process is reduced, because small movements with the mouse pointer will significantly change the selected percentage. Furthermore, the gray bars that are currently placed between the buttons would have to be included into the bullet chart as well. This would increase the complexity of the bullet charts and the decision was made to keep the decision tool separate.

In order to increase the usability, a suggestion was made to add a “cancel“ button alongside the “undo“ and accept button that reverts all changes to the initial state. This removes the need to click the “undo“ button multiple times if desired to do so.

Process insight generation: The goal to **create process knowledge** aims to explain the relationship from the inputs to the process variables to the resulting indicators. The experts voiced their opinion that the understanding of the relationship from inputs to the indicators is key to create acceptance. As a result of their experience, plant managers and operators already have a mental model of the process. Offering information about the entire causal chain allows them to compare their model with insights generated by the DSS. Ideally, this process leads to higher acceptance if the expectation agrees with the findings of the DSS or creates new insights.

While the experts generally agreed that graphs over the course of the reaction are the correct visualization elements, they suggested to arrange them on top of each other to have parallel time axes. Furthermore, the domain experts found the display of reaction rates difficult to understand. Alternatively, a diagram could be used that shows the amount of reaction products in the reactor. Due to the state at the end of the reaction t_f, this representation replaces not only the reaction rates but also the final result, which was represented separately shown by bars. The experts noted that it is sensible to explicitly highlight the process constraints, since the optima are usually on the physical or operational constraints of the process. Another suggestion is to highlight a trajectory if the user hovers over the line and to dynamically show a label that identifies the trajectory or constraint. This is especially helpful when the trajectories corresponding to the newly selected operating point are included as additional lines.

Interface composition: During the last part of the interviews the overall composition of the dashboard's suitability to perform the intended workflow was discussed. Taking into account the findings from before, the experts found that the general composition is difficult to follow, since many different visualization elements were used that are not standard to users of technical systems. Engineers and plant managers think in time series as a standard means of communication of measurements. The implemented reaction rate visualization already gives time series information. However, it only depicts the relative difference between two cases. Thus, the user is not able to extrapolate to the absolute product formation of the individual cases. By providing all the information as trajectories over time, the dashboard is simplified to reduce the cognitive load, also providing the batch output in absolute terms for evaluation. If multiple plots with batch time on the x-axis are used, it is easier to read the plots if consistent axes are aligned.

The experts insisted to keep the functionalities of monitoring, Pareto navigation and process insight in one dashboard to avoid unnecessary navigation across multiple screens. As stated before a good interface should only provide the needed information without cluttering. Asked for a general evaluation of the data classification, the majority of experts considered the reaction equations as less critical information for users that are familiar with the process and suggested to shift the information into a tooltip next to the reactor representation.

The following changes were made to arrive at the final design shown in fig. 5.22: The bullet charts are moved to the top left position and their font size is increased. The table is removed entirely, because the content is also visualized in the bullet charts in connection with the decision tool. The reactor schematic is cleaned up by removing the coloring of the input and output streams. Furthermore, the feed label is updated to explicitly show that only the raw material B is added in semi-batch fashion. The causal chain at the bottom is replaced by time series plots at the right side on top of each

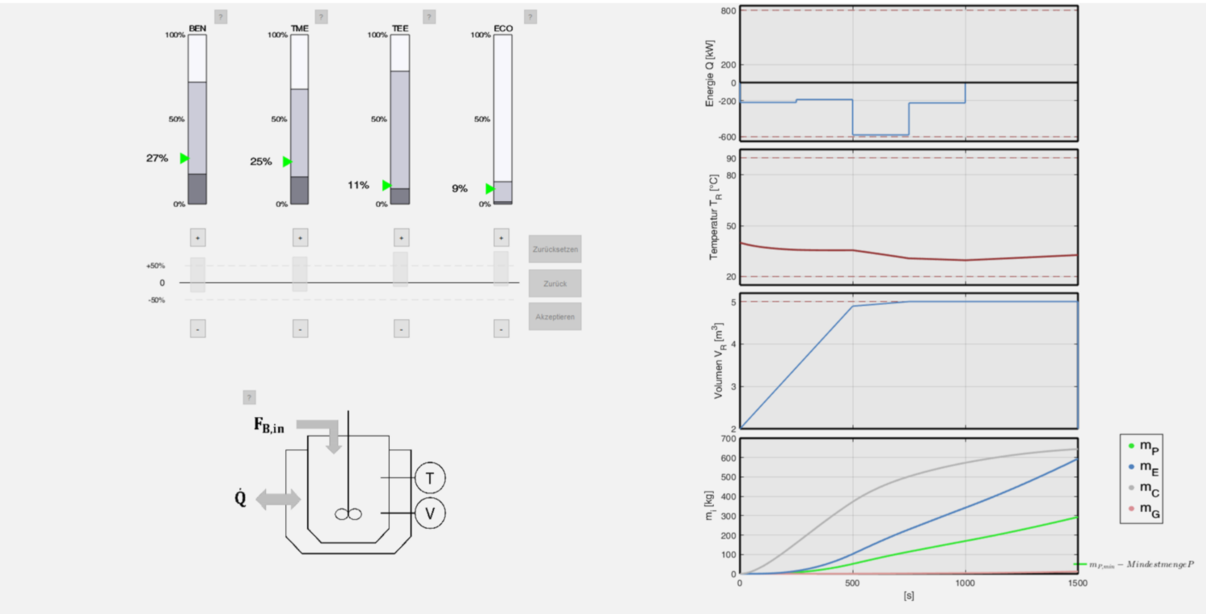


Figure 5.22: Final interface design, before user interaction, with the monitoring and selection elements (top left), the process trajectories (right), and a reactor schematic (bottom-left).

other, from top to bottom: (1) the heating and cooling profile, (2) the reactor temperature (3) the reactor volume, and below the resulting trajectories of species in one plot (4).

Thus, now the upper left corner comprises the monitoring and navigation functionality in one element. The right hand side is dedicated to the process trajectories to cater to the need for process understanding. Some of the information displayed before was now shifted into tooltips that either show when hovered over one of the question marks or over the actual visualization elements in case of the process constraints.

5.4.4 Functional implementation

The dashboard was implemented with the GUIDE tool using MATLAB® 2017b. The updated navigation tool implementation uses an adjusted color coding on the bullet chart axis (cf. 5.23).

Each of the three segments in the bullet charts (black, gray and white) represents a third of the obtained Pareto-points on the indicator scale. Under the assumption that the points are evenly distributed on the frontier, the user can assess if the frontier is wide or narrow for good indicator values. For the given case, the white segment for ECO efficiency is ranging from approximately 15% to 100%. Thus, two thirds of the Pareto-frontier exhibit an ECO efficiency below 15% and it is likely that the degrees

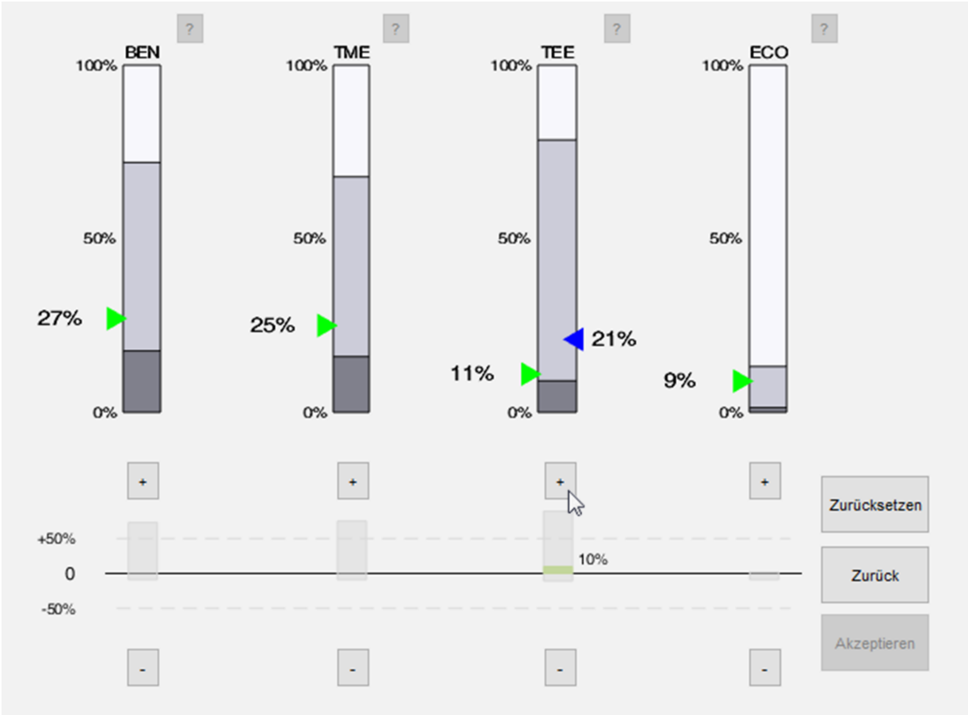


Figure 5.23: Intermediate state of the selection tool after interaction on the energy efficiency performance (TEE).

of freedom are limited for operating points with good ECO efficiency. Below the bullet charts, the selection tool is implemented with similar functionality, where the possible operating points are indicated by the gray ranges that are updated for all indicators upon every user interaction. The group of buttons on the right side is extended by another button that resets the entire selection. Furthermore, all buttons are visible from the start and only grayed out if they are set to inactive. Since, the users are German native speakers, the buttons are labeled in German language. Since the Pareto frontier consists of a number of distinct solutions, in contrast to an approximation, an additional margin must be introduced to allow for smooth navigation, because fixing one indicator at the exact value would constrain the set of remaining points too narrowly. To elucidate this need, we consider an example: if the Pareto frontier is a three dimensional plane, fixing one of the coordinates will reduce the Pareto-front to a line. Now, if we only consider points exactly on this line, it is highly unlikely that a large number of points will remain. Thus, a margin needs to introduced to allow for movement along the line. Furthermore, it is not possible to interpolate between solutions, since trajectories and required inputs are not available for the graphs. Practically this means, that if the user selects e.g. 95.0% efficiency for the BEN indicator, all points with an BEN indicator between 94.0 and 96.0% would remain in the pool of solutions. This approach introduces a necessary inaccuracy to the selection that is still reasonable, because it is in the range of an expected plant-model mismatches for applications in the field of chemical and biochemical engineering applications. Upon interaction with the third value, a unique operating point is selected and the corresponding updates to the rest of the dashboard are made. The indicator definition is available as tooltip next to each bullet chart (cf. fig. 5.24). The question mark fields were implemented as disabled buttons, since they already have an automatic listener implemented that triggers a callback routine as soon as the cursor hovers over the button.

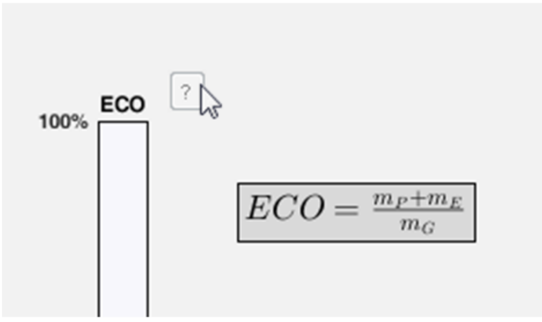


Figure 5.24: Tooltip for the ECO indicator definition.

The trajectories are plotted with the MATLAB® plot functionality as a line plot. Here, it is difficult to distinguish the trajectories due to the piece-wise constant input, because only horizontal lines appear (see fig. 5.25). As soon as the cursor is within the plots the position is tracked and the vertical distance to all trajectories included in the figure is calculated. The closest one is highlighted by a colored polygon (see 5.25, bottom). The polygon is colored either red or blue, depending if it is above zero depicting heating or below depicting cooling. It is partially transparent to avoid a blocking of underlying trajectories.

All constraints on the manipulated and process variables are indicated by a dotted red line (cf. figs. 5.25 and 5.26a). Tooltips are implemented to identify the constraint value as shown in fig. 5.26a. Here, the tooltip is triggered if the distance of the cursor to the constraint is below 10% of the permitted variable range.

The tooltip displayed in fig. 5.26b for the reaction equations is available next to the reactor schematic and is again implemented by a button related callback function.

Finally, the evolution of the species formed in the reaction is plotted in the lowest graph, see fig. 5.27. The raw materials A and B were neglected for clarity, since their consumption can be extrapolated from the (intermediate) product formation. Highlighting as well as color coding is most important in this graph, because after the selection there are eight lines to be considered. To ease the interpretation, the label identifying the currently highlighted compound is shown centrally as a tooltip. Furthermore, an extension of the legend on the right hand side comprehensively shows the direction of change using arrows. Again, the line to highlight is chosen based on the cursor location in the plot.

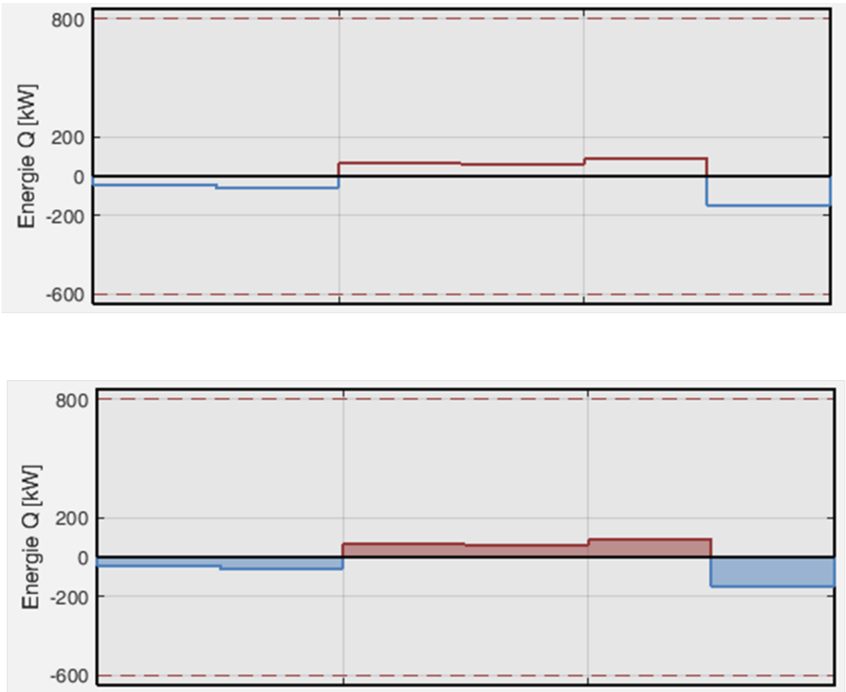
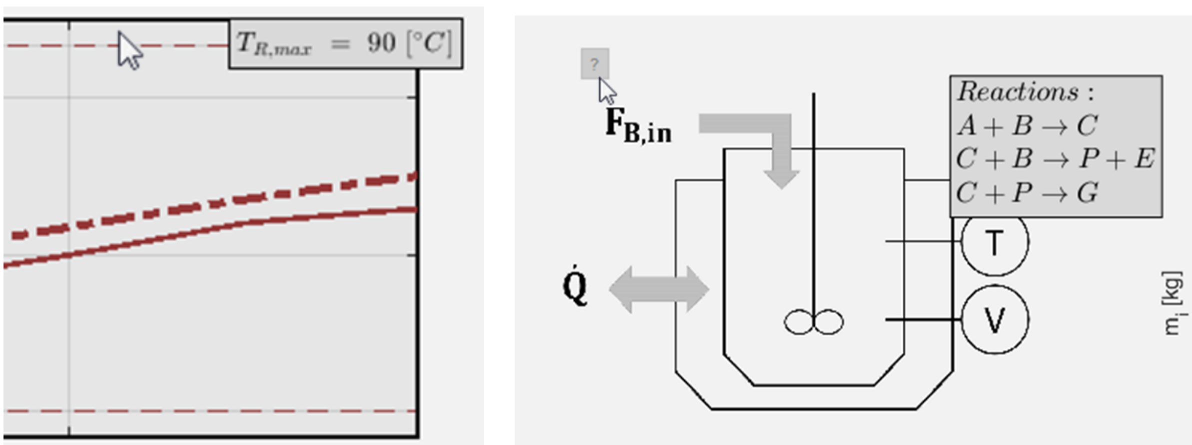


Figure 5.25: Input trajectory for the heating and cooling duty over the course of one batch. Top: static presentation, bottom: highlighted version following the interaction with the mouse.



(a) Tooltip for the upper reactor temperature constraint.

(b) Tooltip for the reaction system, situated next to the reactor sketch.

Figure 5.26: Explanation of the implemented tooltips.

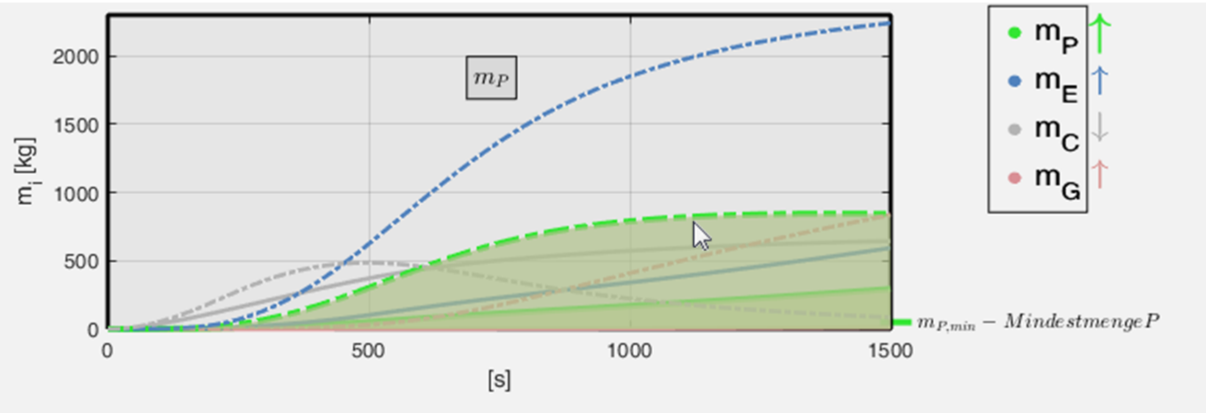


Figure 5.27: Tooltip for the mass trajectory of product P upon user interaction with the mouse. The right hand side indicates the lower endpoint constraint on product P and a legend including the relative change between the current and previous operating point.

5.5 Conclusions

Based on the ecological interface design methodology, this chapter presented an approach to provide efficient decision support solutions for indicator-based resource efficiency optimization of chemical and biochemical production processes. The skill, rule and knowledge framework, which allows a classification of the decision processes according to the required mental resources was found to be a helpful concept. The goal is to preprocess the information as much as possible and to lower the load on the user. Rasmussen (1983) distinguishes between summaries and exceptions to do so. Summaries are, in this case, the REIs, which relate the relevant variables for the efficiency and, compared to a reference value like the Pareto front, directly indicate a conclusion about the efficiency of the process. Exceptions are undesired deviations, which are pointed out to the user, so that he or she can concentrate on the currently relevant situations. The design process described in section 5.3 defines a structured approach to arrive at a system design which optimally supports the decision process. Depending on the desired range of functions, the design process can reach three different stages of development. The least effort, but also smallest benefit, comes from plotting efficiency indicators based on historical production data against the best efficiency ever observed. For the further stages, a sufficiently good model is required. It can be used to obtain the Pareto front by offline optimization. The effort involved is high and results in a continuous maintenance effort to keep the model up to date. Such an effort is only justified for processes with a high resource input, or for individual process sections that are the main consumers of resources. If this effort is made, it can be ensured that the process is operated at or near the actual optimum. In this way, potentially better operating points can be found that were not yet known to the operating team, leading to larger savings. In addition to solely delivering the optimal inputs and achievable efficiencies, the most enhanced version of REI decision support additionally delivers information to understand why the advice will yield the desired outcome. Thus additional insight into the system dynamics is gained, and confidence in the results of the decision support system is created.

After deciding how comprehensive the decision support should be, the selection and composition of the visualization elements is crucial for the quality of the solution. It requires the use of the best visualization elements to display indicators and secondary information. Suitable visualization elements were collected in section 5.2.2 to select the appropriate elements according to the type of information presented. The quality of the solution should be evaluated before the widespread use of the system. Interviews with domain experts and user acceptance tests are suitable for this purpose.

Finally, the framework was successfully applied to the WOSBR example in section in 5.4. The initial dashboard design was based on the analysis of REI visualization elements in section 5.2.2 and was evaluated in expert interviews with chemical and biochemical engineers. The displayed information was minimized to achieve a concise design, while including all information that is necessary to make an informed decision. The following Chapter (Ch. 6) presents the usability evaluation of the resulting DSS by means of a usability study and aims to validate the design.

Chapter 6

Usability Study: decision support for the operation of the Williams-Otto semi-batch reactor

Jens Ehlhardt recruited the study participants and supervised the experiments as part of his duties as student assistant, while the experimental design and interpretation of the results was done by the author.

The goal of this work is to provide guidelines how to realize decision support for the optimization of resource efficiency for batch and semi-batch plants in the process industry. First, a framework for the definition, calculation and presentation of REIs was developed, which can capture the technical performance of production processes in terms of resource efficiency (Chapter 3). Chapter 4 described a procedure to solve the arising multidimensional optimization problem and obtain the set of Pareto optimal operating points for the WOSBR example. Based on the Pareto set, Chapter 5 derived a decision support system that helps the user to select a Pareto-optimal point. The design process was demonstrated using the WOSBR example with four performance metrics. This Chapter investigates the quality of the resulting decision support solution by means of a usability study that evaluates the performance for the following two functionalities:

Function 1: Support for the selection of a new operating point based on the desired performance by navigation on the Pareto front

Function 2: Explanation of the relationships between the operational degrees of freedom and the resulting performance characteristics.

The standard ISO9241-11 states the definitions and concepts of usability for systems, products and services. The methods and evaluation guidelines are derived from a central definition:

> "**usability:** extent to which a system, product or service can be used by specified users to achieve specified goals with effectiveness, efficiency and satisfaction in a specified context of use" (ISO9241-11).

In this case, the usability study covers a system. The standard defines systems as follows:

> "**system:** combination of interacting elements organized to achieve one or more stated purposes
>
> **interactive system:** combination of hardware and/or software and/or services and/or people that users interact with in order to achieve specific goals" (ISO9241-11).

Thus, when evaluating the usability, all constituent parts of the DSS are under investigation, including the user, the dashboard, the calculation routines, and their interactions. This can be achieved by supplying realistic tasks to the study participants and evaluating the outcomes of the decision making process. The usability of a system always has a subjective component that depends on the individual preferences of the users. The personal assessment of the study participants can be recorded by a questionnaire at the end of the experiment and can be compared with objective variables such as the error rate and the average processing time that were recorded during the experiments. The first research question (**RQ**) is formulated accordingly:

> **RQ A – Usability evaluation:** Does the decision support system designed in section 5.4 achieve a high usability regarding the two functionalities of Pareto navigation and explanation of the process interrelations?

The design process was based on considerations from the ecological interface design (EID) and skill, rule and knowledge (SRK) framework, which aim at minimizing the cognitive effort to keep error rates and processing times low. Thus, a second goal of this chapter is to evaluate whether the considerations based on the SRK-framework are valid. Here, the idea is to compare the performance on tasks that were assigned to different SRK categories and evaluate if the performance varies accordingly. An improved understanding of the cognitive effort related to decision making processes in resource efficiency optimization delivers valuable insights for further improvements in the field. Thus, the second research question is formulated:

> **RQ B – Design concept evaluation:** Does the categorization of decision making processes according to the SRK-framework align with the observed impacts on the performance of the decision making process?

6.1 State-of-the-art

After the design process, a quality assessment of decision support systems is often conducted by a usability study. According to the ISO9241-11, usability covers aspects of the entire user experience of integrated human-machine systems:

- Effectiveness, as defined by the ability to perform the task with the desired outcome
- Efficiency, indicated by the resources and time to perform the task
- Satisfaction, a subjective entity reflecting the user's acceptance and motivation to use the solution within the intended application domain

Usability studies should address all three points, because they are dependent on each other to a certain extent. On the one hand, effective and efficient interfaces tend to create a satisfactory user experience, on the other hand the decision support solution will not create a sustainable impact in the long run, if the users experience the interface as cumbersome to use. Effectiveness and efficiency can be objectively recorded through practical experiments. The user satisfaction, however, is highly subjective and depends on the individual user. Within this work, experiments were conducted that recorded objective measurements for effectiveness and efficiency. In conjunction to the experiments, a standardized questionnaire was distributed afterwards that aims to quantify the user experience from a personal point of view. Section 6.1.1 introduces the system usability score (SUS) that is a widely used tool to assess the subjective side of a systems usability.

In the course of the experiments, the processing time and error rates are recorded as objective variables in order to test the working hypotheses. It is necessary to test if there is a statically significant difference between the comparison groups. If so, the varied variable has an influence on the recorded performance. In statistics, a distinction is made between parametric and non-parametric tests (Moore, 2009). Parametric tests are generally characterized by a higher sensitivity, but make some assumptions about the population of scores that have to be fulfilled. One of the assumptions is a normal distribution of the measurements, which cannot be upheld for the processing time and error rate, because the range of values is limited to the positive range and is mostly skewed towards zero. Thus, in the context of this work the non-parametric "Kruskal-Wallis test" is used, which is also suitable for the comparison of different sample sizes (Kruskal and Wallis, 1952). It is described in 6.1.2.

6.1.1 System usability score (SUS)

The system usability scale (SUS) was developed by Brooke (1996) to measure the general usability of a technical system at low-cost. The assessment is based on a survey that targets the topics, efficiency, effectiveness and user satisfaction, with the statements listed in tab.

6.1. The users have to respond by rating each statement on a scale from one to five, where one represents "I strongly agree" and five "I strongly disagree". The discretization of the scale is one, thus no partial points can be awarded. To avoid anchoring of the responses towards one end of the scale, the orientation of a positive assessment is alternating. The SUS for each survey is calculated by equation 6.1, where P_i is the number of points awarded in question i. The overall score SUS_{total} is on the interval $[0, 100]$.

$$SUS_{odd} = \sum_i P_i - 1 \qquad \forall \; i \in \{1,3,5,7,9\} \tag{6.1a}$$

$$SUS_{even} = \sum_j 5 - P_j \qquad \forall \; j \in \{2,4,6,8,10\} \tag{6.1b}$$

$$SUS_{total} = 2.5 \cdot (SUS_{odd} + SUS_{even}) \tag{6.1c}$$

Table 6.1: Questions according to SUS-questionnaire (Brooke, 1996), German translation is provided in the appendix C

Number	Question
1.	I think that I would like to use this decision support tool frequently
2.	I found the decision support tool unnecessarily complex
3.	I thought the decision support tool was easy to use
4.	I think that I would need the support of a technical person to be able to use this decision support tool
5.	I found the various functions were well integrated
6.	I thought there was too much inconsistency in this decision support tool
7.	I would imagine that most people would learn to use this system very quickly
8.	I found the system very cumbersome to use
9.	I felt very confident using the system
10.	I needed to learn a lot of things before I could get going with this system

In literature a SUS score of 63 is often reported as the lowest acceptable. Bangor et al. (2009) investigated how the SUS aligns with other measures used to grade the usability of a system. Figure 6.1 relates the SUS score to acceptability ranges, the grade scale and adjective ratings as reported in literature. Within the scope of this theses the goal regarding usability is to achieve a SUS score above 70, which translates to a performance of A, B or C on the grade scale and adjective ratings of at least good.

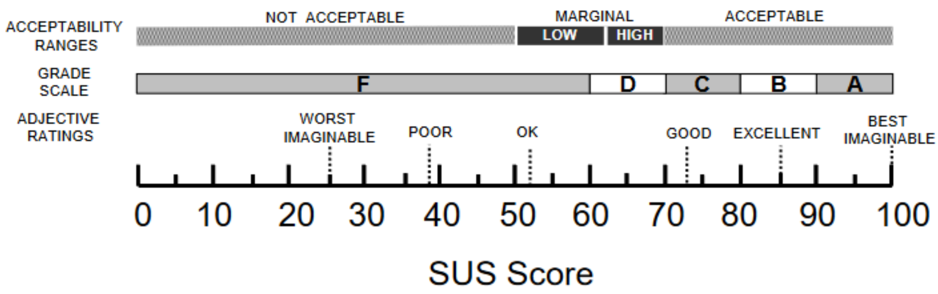


Figure 6.1: Alignment of the SUS score with other usability assessment scales. Taken from Bangor et al. (2009).

6.1.2 Kruskal-Wallis test

The experimental investigation regarding the efficiency and effectiveness of REI-based decision support is done by testing hypotheses that formulate a statement regarding the correlation between a suspected influence and the target measure. In the experiments, the influence is varied across two or more groups, while recording the performance measures. Then, the Kruskal-Wallis test is used to validate or disprove the hypothesis by comparing the performance for the groups. Generally, the hypotheses are formulated as a null hypothesis:

“The statement being tested in a test of statistical significance is called the null hypothesis. The test of significance is designed to assess the strength of the evidence against the null hypothesis. Usually, the null hypothesis is a statement of 'no effect' or 'no difference'.”(Moore, 2009) The null hypothesis is symbolized by H_0.

The Kruskal-Wallis test, also known as H–test, is a non-parametric statistical test that either leads to the acceptance or rejection of the null hypothesis H_0, which states that the scores of two or more samples are drawn from the same or equivalent populations (Kruskal and Wallis, 1952; Howell, 2010). The population is a collection of observations that were recorded to confirm or refute the hypothesis. In order to investigate the effect of one influence or characteristic on a numeric performance measure, the influence is varied among different subsets of the population, called samples. The outcomes on the performance measure are called scores. In case the influence does not have an effect on the performance measure the null hypothesis holds and the samples originate from the same or an equivalent population. There are no assumptions made regarding the overall population and samples. Thus, the test is also suitable for data whose residuals are not normally distributed. The Kruskal-Wallis test is particularly sensitive to differences in the central tendency or median (Howell, 2010).

It does not consider the scores directly in the statistical evaluation, but the rank of each score regardless of their sample affiliation. Hence, the first step is to rank all scores in ascending order. If there are multiple scores with the same value they are assigned with the average rank across the sample of identical scores. The test statistic H is given by equation 6.2, where N is the total number across all k samples, n_i the number of scores within the samples, and R_i the sums of rank in each sample.

$$H = \frac{12}{N(N+1)} \sum_{i=1}^{k} \frac{R_i^2}{n_i} - 3(N+1) \tag{6.2}$$

H is a direct measure of the degree to which the R_i differ across the samples. The H-metric is compared to critical values H_c as provided in Kruskal and Wallis (1952). If the calculated value for H is found to be smaller than the critical value, the null hypothesis is accepted, otherwise rejected with at least one sample being significantly different to the others. For large sample sizes ($n_i \geq 5$) the probability distribution of H is identical to the χ^2–distribution that is more readily available and easier to calculate (Howell, 2010). The parameters needed to obtain the critical values from the χ^2–distribution are the significance value α and the degrees of freedom $df = k - 1$.

Example case

In order to illustrate the statistical tests described in 6.1.2, they will be performed for an exemplary data set taken from (Howell, 2010) that is fictional, but designed to meet the means and variances of the original study published by Eysenck (1974). Eysenck studied the level of recall for words that were memorized using different techniques namely counting, rhyming, adjective, imagery, and intentional. For each sample of treatment ten scores were recorded as shown in table 6.2.

The null hypothesis H_0 for both cases is the statement: There is no difference in the level of recall across the five samples that were subject to different learning strategies.

First, the one-way ANOVA test will be performed, by calculating the F–value (eq. 6.5) based on MS_{error} and MS_{treat} (eqs. 6.3 and 6.4). The data set under investigation meets the necessary assumptions for the one-way ANOVA test (Howell, 2010).

$$MS_{error} = \sum_{j=1}^{5} \frac{s_j^2}{k} = (3.33 + 4.54 + 6.22 + 20.27 + 14.00)/5 = 9.67 \tag{6.3}$$

$$\begin{aligned} MS_{treat} = ns_{\bar{X}}^2 &= \frac{n \sum_j^k (\bar{X}_j - \bar{X}_{..})^2}{k-1} \\ &= \frac{(-3.06)^2 + (-3.16)^2 + (0.94)^2 + (3.34)^2 + (1.94)^2}{5-1} = 87.88 \end{aligned} \tag{6.4}$$

$$F = \frac{MS_{treat}}{MS_{error}} = \frac{87.88}{9.67} = 9.09 \tag{6.5}$$

Table 6.2: Data from Howell (2010) in accordance with Eysenck (1974). Listed are the scores of the participants in the respected learning samples. In parenthesis the ranks for the Kruskal–Wallis test are listed (Kruskal and Wallis, 1952).

	Counting	Rhyming	Adjective	Imagery	Intentional	Total
	9 (21)	7 (10.5)	11 (32.5)	12 (38.5)	10 (25)	
	8 (14.5)	9 (21)	13 (41)	11 (32.5)	19 (48.5)	
	6 (8)	6 (8)	8 (14.5)	16 (47)	14 (44)	
	8 (14.5)	6 (8)	6 (8)	11 (32.5)	5 (3.5)	
	10 (25)	6 (8)	14 (44)	9 (21)	10 (25)	
	4 (2)	11 (32.5)	11 (32.5)	23 (50)	11 (32.5)	
	6 (8)	6 (8)	13 (41)	12 (38.5)	14 (44)	
	5 (3.5)	3 (1)	13 (41)	10 (25)	15 (46)	
	7 (10.5)	8 (14.5)	10 (25)	19 (48.5)	11 (32.5)	
	7 (10.5)	7 (10.5)	11 (32.5)	11 (32.5)	11 (32.5)	
Mean	7.00	6.90	11.00	13.40	12.00	10.06
St. Dev.	1.83	2.13	2.49	4.50	3.74	4.01
Variance	3.33	4.54	6.22	20.27	14.00	16.058

Here, $\bar{X}_j$ is the mean per memorizing technique and $\bar{X}_{..}$ the grand mean. The F–distribution value for a significance value $\alpha = 0.05$, the degrees of freedom for the numerator $df = k - 1 = 4$, and the degree of freedom for the denominator $df = k(n-1) = 45$ is $F_{0.05}(4, 45) = 2.58$. Since, the calculated F–value is larger than $F_{0.05}(4, 45)$ the null hypothesis is rejected according to the results of the one-way ANOVA.

The Kruskal–Wallis test as outlined in section 6.1.2 is based on the sum of ranks for all observations within each sample according to the H-metric (see eq. 6.6).

$$
\begin{aligned}
H &= \frac{12}{N(N+1)} \sum_{i=1}^{k} \frac{R_i^2}{n_i} - 3(N+1) \\
&= \frac{12}{50(50+1)} \left(\frac{122^2}{10} + \frac{312^2}{10} + \frac{366^2}{10} + \frac{333.5^2}{10} \right) - 3(50+1) \\
&= 21.69
\end{aligned}
\tag{6.6}
$$

The resulting H–value is referenced against the χ^2 value for a significance level of $\alpha = 0.05$ and degrees of freedom $df = k - 1 = 4$, which is equal to 9.49. Since, H is larger than the χ^2–value the null hypothesis is also rejected based on the Kruskal–Wallis test (Howell, 2010).

6.2 Experimental design and procedure

The two functionalities of the DSS require different types of interaction: Function 1 includes a selection process and requires two-way interaction. The second function that is generating process knowledge requires only passive perception and information processing. To investigate how well the system performs, two types of tasks are used during the experimental study. All participants will answer the full set of questions for both types, in order to obtain comparable results. Alternating the type of tasks and randomizing the order ensured that systematic effects are excluded.

Type 1 - Pareto navigation trials

The first type of experimental trials simulates the selection process. The user is tasked to interact with the MATLAB® implementation of the interface to select a new operating point on the Pareto-frontier that meets given requirements. Each user is given a total of 40 type 1 trials with varying starting points and target requirements. The new operating point is selected by pressing the buttons below the bullet charts that change the corresponding indicator. The selection can be accepted as soon as the target requirements result in a unique point. Each task is displayed in a field at the lower left of the screen (c.f. fig 6.2).

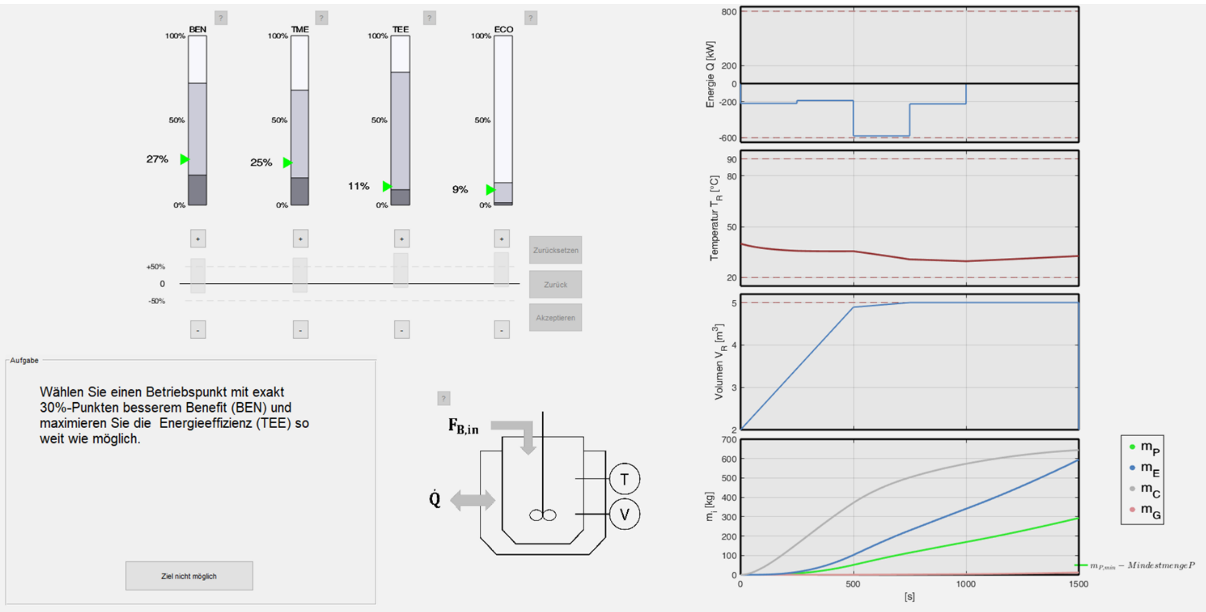


Figure 6.2: Experimental setup during type one trials. The trial task is displayed in lower left corner.

A total of 32 tasks were feasible, whereas eight of them were impossible to achieve. In the former case, the trial was registered as successful if the user pressed the accept button and an operating point was selected that met the requirements. In the latter case, the trial was recognized as solved correctly if the user clicked the button “not possible”. Furthermore, the time on task was recorded to evaluate how efficient the user performed the task. The entire set of trials did not require any input via the keyboard. Hence, the only means of input given to the participants was a standard computer mouse. Each interaction with buttons or tooltips was recorded as supplementary information.

Type 2 - Understanding trials

The second type of tasks is dedicated to test if the dashboard adequately explains the interrelations from process inputs to resource efficiency. For a total number of 40 trials, each user selects the correct statement among three alternatives (cf. fig 6.3). For each trial the result of a Pareto selection process is shown, including the previous operating point and the newly selected operating point. Only one of the statements is correct and needs to be selected by clicking on the corresponding radio-button and subsequently clicking “OK”.

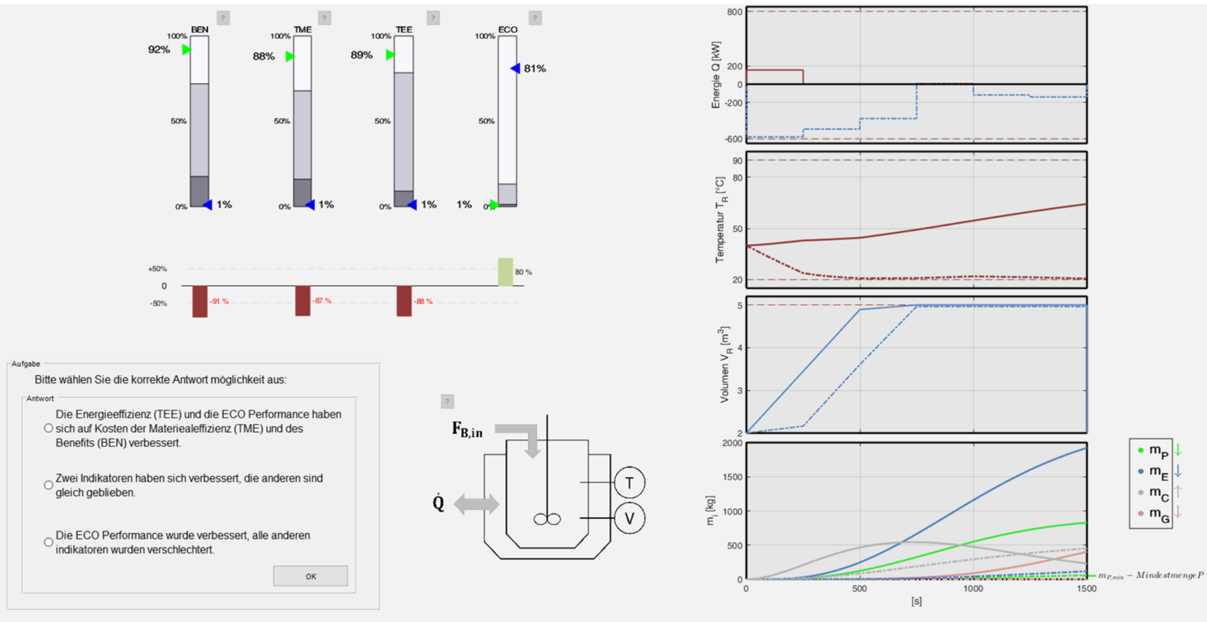


Figure 6.3: Experimental setup during type two trials. The bullet charts indicate the efficiency of the previous operating point with green triangles and the final selection with blue triangles. The time series plots differentiate the trajectories with solid (previous) and dashed lines (final selection).

Again, the time-on-task and given response are recorded to determine the performance metrics. Since the user does not need to use the buttons, only tooltip interactions were recorded as supplementary information.

6.2.1 Usability evaluation (RQ A)

RQ A is concerned with the usability of the decision support system with respect to the Pareto navigation and insight generation functionalities. ISO9241-11 lists three key metrics to evaluate the usability: effectiveness, efficiency, and satisfaction and defines them accordingly:

> "**effectiveness:**
> accuracy and completeness with which users achieve specified goals
>
> **efficiency:**
> resources used in relation to the results achieved
>
> **satisfaction:**
> extent to which the user's physical, cognitive and emotional responses that result from the use of a system, product or service meet the user's needs and expectations" (ISO9241-11).

Effectiveness
Function 1 of the DSS is considered effectively solved if an operating point is selected that fulfills the task requirements or if the user correctly identifies the task as impossible to solve. For example, this can be the case if the task requires a high level of benefit alongside a highly ECO efficient operation. The second functionality is considered to be effectively solved if the correct statement among three alternatives is selected. The assessment of the resulting error rate per function is an objective measure of the DSS's effectiveness. The ultimate target of the DSS is to improve the resource efficiency of production processes by choosing an operating mode on the Pareto frontier that meets the performance objectives of the user. However, since the optimization of resource efficiency is not a safety critical decision making process, a low failure rate is acceptable as it only results in the selection of another Pareto optimal operating point. But, in order to achieve a sustainable improvement of resource efficiency, the target for the error rate is below 10%.

Efficiency
According to the ISO9241-11 efficiency is defined by the relation of the used resources to the achieved result. In the case at hand the only resource spent during the use of the DSS is the time invested by the user. Thus, the time span between showing the task to the moment an answer is registered can be used as an objective measure of efficiency. Generally, the importance of the systems efficiency increases with the frequency of use. In an industrial setting, the DSS would be used right after it's implementation and every time the user preferences regarding resource efficiency or economic performance change.

The frequency of use is approximated as once or twice a month. Thus, a period of up to five minutes for the selection of an operating point and understanding the inner relationships is deemed reasonable.

Satisfaction – Learnability
Satisfaction is difficult to evaluate using objective measures, since there is always an individual element to the user experience. A factor enabling user satisfaction, however, is the learnability of a system that is new to the user. After a brief user training, the participants of the study interacted with the DSS for the first time during the experiment. Therefore, it was interesting to study the initial learning curve over the course of the experiment. The learning effect is expected to impact the performance regarding the time-on-task towards the end of the experiment for both functionalities. A good learnability is expected to translate to a decrease of the time-on-task. Thus, for each type the responses of all participants are divided into two sets that comprise the first half ("start"-set) and the second half of the responses ("end"-set). Then the performance measures for both sets are tested for significant differences. To statistically evaluate the assumption, the following null hypotheses are formulated.

Hypothesis 1 (H1): *There is no learning effect during type 1 trials, thus the time-on-task for the first half of the experiment is not significantly different from the recorded time-on-task for the second half of the experiment.*

Hypothesis 2 (H2): *There is no learning effect during type 2 trials, thus the time-on-task for the first half of the experiment is not significantly different from the recorded time-on-task for the second half of the experiment.*

Table 6.3 lists the independent and dependent variables for hypothesis H1 and H2. The independent variables result from the division into two sets, whereas the dependent variables are automatically recorded during the trials. In order to assess if the independent variables have a significant influence on the dependent variables, it is necessary to test both hypotheses using the Kruskal-Wallis test. Since all dependent variables are numeric values and measurable on a continuous scale, the objective of the tests will be to determine if the results of distinct groups originate from the same population. By design the test groups are defined according to the independent variables. Thus, if the test identifies a difference between two groups, we conclude that the change in the independent variable was the likely cause of the change of the dependent variable. Here, the hypotheses assume that there is no difference between the respective "start"- and "end"-sets, which would suggest that they originate from the same population. In case the hypotheses are rejected on the basis of a suitable significance test, the assumption of a learning effect is confirmed.

System Usability Scale survey
The System Usability Scale (SUS), according to Brooke (1996), is an established tool

Table 6.3: Overview of relevant hypotheses with the corresponding independent and dependent variables.

Hypothesis	Independent Variable	Dependent Variable
H1: Learnability of the selection interface	experience with the interface: start-/end-set	time-on-task
H2: Learnability of the insight generation	experience with the interface: start-/end-set	time-on-task

to quantify usability using a standardized survey. It contains questions that aim at all three factors of usability: effectiveness, efficiency, and satisfaction. Details about the SUS can be found in section 6.1.1, and the appendix C.1 lists the German translation of the questions from tab. 6.1 that were given to the participants after the completion of the experiment. Care was taken to preserve the alternating orientation in the formulation of the questions to prevent any anchoring toward one end of the scale. This means that a positive assessment is on alternating ends of the scale. The target DSS under investigation is to score in the acceptable range equal or above 70 (c.f. fig. 6.1).

6.2.2 Design concept evaluation (RQ B)

The design of the DSS was based on considerations regarding the SRK-framework. Depending on the difficulty of the tasks, the decision making process falls under different categories, the skill, rules or knowledge level. Decisions on the skill level do require the least amount of cognitive effort, since the user directly knows how to react to a certain situation. For decisions made on the rule-based level the user needs to apply a set of rules to the problem in order to find the correct response to a task. If the user needs to rely on experience and deeper system knowledge to choose the appropriate response, the knowledge-based level is reached that requires the largest cognitive effort. According to the framework, an increased cognitive effort is associated with an increased probability of mistakes and increasing time needed to solve the task.

A well-designed DSS prepares the decision-making process by pre-processing necessary information and presenting it in an understandable way. This makes it possible to reduce decision processes from a knowledge- or rule-based level to a cognitively less demanding level. In the case of resource efficiency optimization, the calculation of the indicators defined in section 4.2.2 and the multi-criterial optimization in section 4.2.3 represents this pre-processing. The considerations in section 5.4 aimed at composing the correct visualization elements to create an easy to understand user interface that can be interpreted quickly and with low error rates.

In order to verify the underlying assumptions of the SRK-framework and their implications for the developed DSS, the trial tasks for the Pareto navigation (function 1) and insight generation (function 2) are divided into three levels of difficulty. The tasks in each category are chosen to be subject to the same classification according to the SRK-framework. Thus, a statistical comparison of the group's performance with regard to efficiency and effectiveness allows to subsequently evaluate whether the classification into different SRK levels has the expected impact. In order to prevent systematic influences, the order of tasks is randomized for each participant.

Type 1 - Pareto navigation

The differentiation between categories of complexity aims to investigate how severe the complexity of the tasks impacts the performance metrics. The complexity is determined by the number of requirements stated in the task. In the case of the Pareto navigation the decision making process is either skill- or rule-based, because the pre-processing of information made knowledge-based decision making obsolete. The three categories are:

Category 1 - easy: The user is tasked to either maximize one of the indicators, to choose an operating point that exhibits a specific efficiency on one indicator or to increase the efficiency on one indicator by a given amount of points. The user can directly manipulate the corresponding indicator using the buttons below the bullet charts. Thus, the process is skill based and expected to perform best compared to the other categories.

Category 2 - medium: Here, the task specifies requirements on two indicators that need to be fulfilled with the prospective operating point. The requirements request an indicator to be greater than a threshold, to be improved by an exact amount, to achieve a specified efficiency, or to be maximized. Since trade-offs between the indicators are present, the decision making process is rule-based and the user must check for compliance of the requested performance on two indicators. Depending on the sequence of manipulated indicators it is necessary find the solution iteratively or realize that the requested combination of performance measures is not achievable. Compared to category one, the performance regarding efficiency and effectiveness is expected to deteriorate. A good DSS design minimizes or eliminates the performance decrease.

Category 3 - difficult: This category of questions imposes constraints on all four of the indicators, with the same type of constraints as listed under category 2. Since only three degrees of freedom are available, constraints on all four can render the task impossible. In principle, the decision making process is also rule-based with an increased number of requirements and rules to follow. Thus, the performance is expected to be on a similar order as category 2 trial tasks. The effect of an increased number of constraints compared to category two trials is expected to have a smaller impact than the shift from skill-based to rule-based decision making.

Type 2 - insight generation

The second function of the DSS aims to explain the cause and effect relationships between the system inputs and the resource efficiency. Again, each participant was presented with the same set of trials, in a randomized order to prevent any systematic interference between trials. In order to prohibit interference with tasks of type 1, both types were alternated in order. The following three categories of questions were distinguished:

Category 1 - easy: In this category, the task was to identify if one of the indicators either improved or deteriorated. The ability to derive this information in a fast and correct manner is a prerequisite to perform any of the intended tasks and hence vital for a successful decision support. The task can be solved instantaneous on a skill-based level by comparing the values indicated on the corresponding bullet chart.

Category 2 - medium: To understand the inherent trade-offs among the different aspects of resource efficiency, the relative orientation of simultaneous change in the indicator values must be inferred from the decision support interface. Thus, trials from category 2 comprise statements of the type: “The energy efficiency (TEE) and the material efficiency (TME) changed in the same direction” or “The benefit (BEN) was improved, while all other indicators deteriorated”. The assessment which of the presented options is correct involves the evaluation of “If-Then” type statements that fall under rule-based decision making. Following the SRK-framework, tasks from this category are likely to result in a reduced efficiency and effectiveness compared to category one trials.

Category 3 - difficult: The third and significantly more complex category includes statements about the causal chain of effects from inputs to process variables or from process variables to changes in the indicator values. To solve this type of task the user is required to evaluate the reaction system, the influence of the temperature on the reaction rates or the definition of the REI. The required knowledge is either already present in the user’s mental model of the process or can be accessed via tooltips in the interface. Either way, deriving the trial response falls under the knowledge-based decision making. Thus, an increased cognitive effort is expected to cause the worst efficiency and effectiveness performance among the type 2 trials. However, a well designed DSS can make the required information easily accessible and reduce the negative impact.

Efficiency of Pareto navigation The cognitive load associated to the completion of the tasks depends on the amount of requirements and REIs that needs to be considered. An increase in the number of constraints will lead to a higher number of interactions and, to some extent, an increase of the time-on-task. The design of the selection interface aims to reduce the cognitive load by pre-calculating the efficiencies and displaying them in an intuitive way. Thus, the desired outcome is no or only little increase in the time-on-task and number of interactions for trials with a different number of constraints and hence difficulty. However, the fact remains that type 1 – category one trials can be answered with skill-based decision making, opposed to the rule-based decision making in case of categories two and three. Hypothesis H3 and H4 are the corresponding null hypotheses that will be used to assess the interaction efficiency.

Hypothesis 3 (H3): *The difficulty of the Pareto navigation task does not have an impact on the response times for type 1 trials. Hence, there is no significant difference between the time-on-task performance, when comparing any combinations of the categories one, two and three of type 1 trials.*

Hypothesis 4 (H4): *The difficulty of the Pareto navigation task does not have an impact on the number of interactions recorded for type 1 trials. Hence, there is no significant difference between the number of recorded interactions, when comparing any combination of the categories one, two and three of type 1 trials.*

Effectiveness of Pareto navigation A high level of accuracy is desirable to achieve effective decision support. The interface aims to make the selection process as easy as possible to reduce the error rate among the trial responses, especially for more difficult trials. With an increase in task complexity it is more likely that inaccurate responses occur. If H5 cannot be rejected for any combination of categories there is no evidence for an influence of the task-complexity on the error rate. If the null hypothesis is rejected there is evidence to support the reasoning that an increase in cognitive effort results in an increased error rate.

Hypothesis 5 (H5): *There is no effect of the task difficulty on the observed error rate for type 1 interaction trials. Thus, there is no significant difference between the error rates, when comparing any combination of the categories one, two and three of type one trials.*

Efficiency of insight generation The main functionality of the interface is to supply the correct inputs to achieve an operating point with the desired efficiencies among the resource efficiency indicators. However, the interface will only achieve a significant impact on resource efficiency if it is regularly used and trusted to give the correct decision support. The option to check the validity is expected to create trust. Part of the interface is dedicated to explain the behavior during the batch and to deliver the information that is needed for validation. The task type 2 trials are set up in three levels of difficulty. If the null hypotheses H6 and H7 cannot be rejected for a comparison between two difficulty groups, there is no evidence to suggest that there is a influence of the tasks difficulty on the measured performance metric.

Hypothesis 6 (H6): *There is no effect of the task difficulty on the observed time-on-task for type 2 understanding trials. Hence, there is no significant difference between the recorded time-on-task, when comparing any combinations of the categories one, two and three of type 2 trials.*

Hypothesis 7 (H7): *There is no effect of the task difficulty on the observed number of interactions for type 2 insight generation trials. Hence, there is no significant difference between the recorded number of interactions, when comparing any combinations of the categories one, two and three of type 2 trials.*

Effectiveness of insight generation The effectiveness of the dashboard for insight generation is measured by the error rate per type 2 trial. A rejection of the null hypothesis H8 when comparing the difficulty levels of type 2 trials indicates that a difference in task complexity also impacts on the error rate. Ideally the error rate should be as low as possible and not increase with task difficulty.

Hypothesis 8 (H8): *There is no effect of the task difficulty on the observed error rate for type 2 understanding trials. Hence, there is no significant difference between the recorded error rate, comparing combinations of the categories one, two and three of type 2 trials.*

Table 6.4 summarizes the hypotheses for the design concept evaluation. During the experiment, the independent variables are systematically varied to study the impact on the dependent variables that are the measures to asses the hypotheses.

6.2.3 Confounding variables

Prior to the experiments, interfering influences need to be anticipated to develop counteracting strategies. Table 6.5 lists the relevant confounding variables and what kind of control strategy is applied. For example, the efficiency of the dashboard is measured by the time-on-task and number of interactions. According to tab. 6.4 the time-on-task is also used in the evaluation of process understanding and learnability. Thus, it is necessary to control the interfering effects statistically and by experimental design. Three difficulty levels are introduced and separately evaluated, while randomizing the order of questions for each participant. Consequently, it is improbable that for example all difficult questions occur at the end of the experiment where the user is more skilled and achieves better scores through the learning effect. Contrastingly, the learning effect is solely evaluated according to the sequence in the list. In relation to the growing process knowledge of the participants, the two types of questions will be alternated to obtain measures on both trial types during each phase of the experiment.

Table 6.4: Overview of relevant hypotheses with the corresponding independent and dependent variables.

Hypothesis	**Independent Variable**	**Dependent Variable**
H3/H4: Efficiency of selection interface	task complexity	time-on-task number of interactions
H5: Effectiveness of selection interface	task complexity	error rate
H6/H7: Efficiency of insight generation	length of causal chain	time-on-task number of interactions
H8: Effectiveness of insight generation	length of causal chain	error rate

Table 6.5: Confounding variables to be controlled during the experiment.

Usability measure	**Confounding variable**	**Control strategy**
Efficiency	**Learning effect** if tasks of different complexity are grouped. Growing **process understanding** over time.	**Control statistically** by randomization of the order of questions for each user. **Control experimentally** by investigating the performance for levels of difficulty
Effectiveness	**Learning effect** if tasks of different complexity are grouped. Growing **process understanding** over time.	**Control statistically** by randomization of the order of questions for each user. **Control experimentally** by investigating the performance for levels of difficulty
Learnability	The **task order** might falsely indicate a learning effect if ordered difficult to easy	**Control statistically** by randomizing the order, also across difficulty levels
Perceived usability	**Individual differences** in user preferences	**Control statistically** by using a suitable number of participants

6.2.4 Subjects

The intended user group of the interface application are plant managers that have the authority to interfere in the process operation of the plant. Due to the lack of accessibility to the user group, 30 university students with engineering backgrounds were selected as participants of the study. All students had an engineering background from the field of chemical and biochemical engineering or engineering economics. Thus, all participants had the competency to understand the process and interpret time series data, comparable to the intended user group. All subjects attended voluntarily and were paid 20 € for the participation in the study.

6.2.5 Procedure

The experiment started with an introduction video of 20min and 58sec and was conducted in German, since all participants were German native speakers.[1].

The introduction was structured in five parts:

1. WOSB process (6:30min)
2. Resource efficiency indicators (2:45min)
3. Multi-criteria optimization (3:00 min)
4. Decision support interface (7:00 min)
5. Experimental setup (1:45 min)

The process introduction (1) walked the subjects through the necessary information to understand the Williams-Otto Semi-Batch Reactor (WOSBR) process. It explained the irreversible reaction equations eq. 4.4–4.6 and identified which of the components are raw materials, intermediate products, value products and waste compounds. Furthermore, the influenceable operational variables were highlighted, while the total batch time is fixed. To complete the introduction, two exemplary batches were explained step by step, based on the relevant trajectories. The batches differed from each other in the amount of cooling supplied to process to show the effects of altered inputs. The introduction of the REIs TME, TEE, ECO and BEN defined in eqs. 4.11–4.14 involved an explanation of the method and the goal of the resource efficiency optimization task (2). Afterwards, the concept of Pareto-optimality (3) was presented by means of a two-dimensional example involving TEE and BEN. Finally, the constituent parts of the interface (4) and their functionality were addressed, concluding in the types of questions to expect during the experiment.

[1]The introductory video is included in the DVD appendix under the filename "Introduction-presentation-final.pptx"

Afterwards each participant was faced with the same set of forty questions from type one and type two each. As stated before, the array of questions alternated between both types and was randomized with respect to the sequence of questions to prohibit any systematic effects. Every interaction with the interface was recorded and timed to obtain the time-on-task, the number and type of interactions with the interface, as well as the validity of the response. Finally, after the conclusion of the experimental part, each of the participants was required to complete a SUS survey with ten questions to subjectively assess the usability of the decision support system.

6.3 Results

The experiments outlined in section 6.2 were conducted with 30 participants. Due to a failing script in one experiment, only 29 were recorded and will be evaluated hereafter. The responses of this user to the SUS survey were included, since the interactions and functionality did execute without problems.

The statistical test used to ascertain differences between trial groups relies on the formulation of a null hypothesis that insinuates that both samples belong to the same population (Kruskal and Wallis, 1952). If the null hypothesis cannot be rejected according to the selected level of confidence there is either no effect or the effect cannot be observed under the variance of the population and samples. Because the dependent variables can only assume values greater than zero, the distribution is skew towards the zero time constraint for most groups. Hence, the assumption of a Gaussian distribution does not hold and prevents the use of most parametric tests. In addition, the group sizes vary, favoring a non-parametric test such as the Kruskal-Wallis test described in section 6.1.2. The Kruskal-Wallis test does not assume a normal distribution and is suitable to evaluate the null hypotheses H1–H8, thus testing wether the groups originate from the same population.

6.3.1 Usability evaluation (RQ A)

Effectiveness

A total number of 1160 trials were recorded for each trial type and assessed regarding the validity of the given responses (see fig 6.4 and 6.5). The observed error rate for type 1 trials is 13.0%, compared to 2.0% in case of type 2 trials. Figure 6.5 further breaks down the error rate per individual question and shows that the distribution is skew towards zero for both trial types. The Pareto navigation trials (type 1) exhibit a mean of 13.4%, while the median is 6.9%. This indicates that the mean is heavily influenced by outliers towards an increased error rate. Indeed, a small number of trials have an error rate above 50% causing the mean to rise. The breakdown of the insight generation trials shows a mean value at 2.1% with a median at 0%, expressing a better performance or a lower level of difficulty.

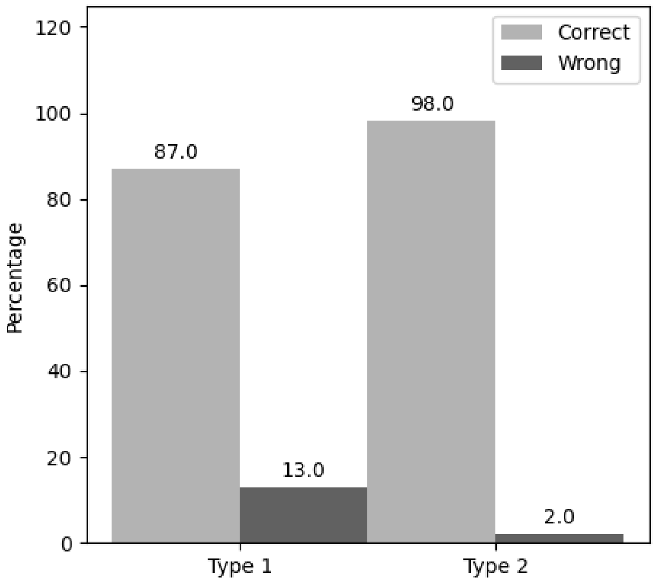


Figure 6.4: Assessment of the error rate regarding type 1 and type 2 trials.

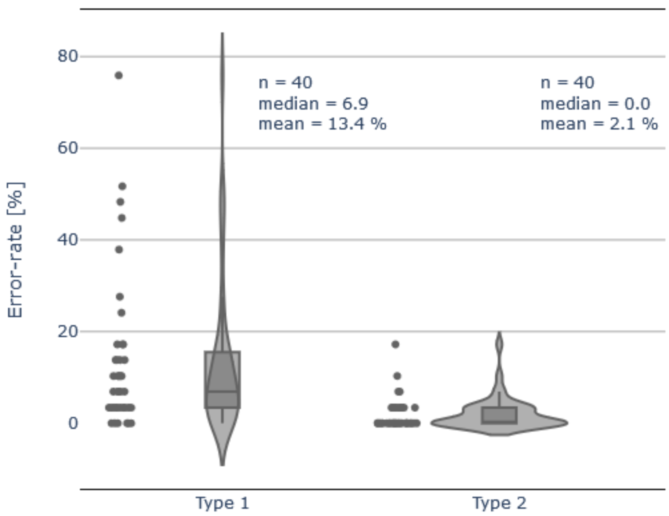


Figure 6.5: Distribution of error rate per trial for type 1 and type 2.

Efficiency

The time-on-task is an objective measure for the efficiency of the DSS and the results for a total of 2320 recorded responses are shown in 6.6. For type 1 trials the users concluded the tasks on average after 34.5s. Again, a lower median of 22.7s indicates a distribution that is skew towards zero. The efficiency regarding insight generation (type 2) is better with an average of 23.9s and a median of 19.0s. The stated objective was to implement a decision support system capable of performing the Pareto navigation and insight generation within $5min$. Awarding two and a half minutes or $300s$ to each functionality, the mean time-on-task for both functionalities is well below the target. Furthermore, only 1.5% and 0.08% of the responses violated the target for type 1 and type 2 trials respectively.

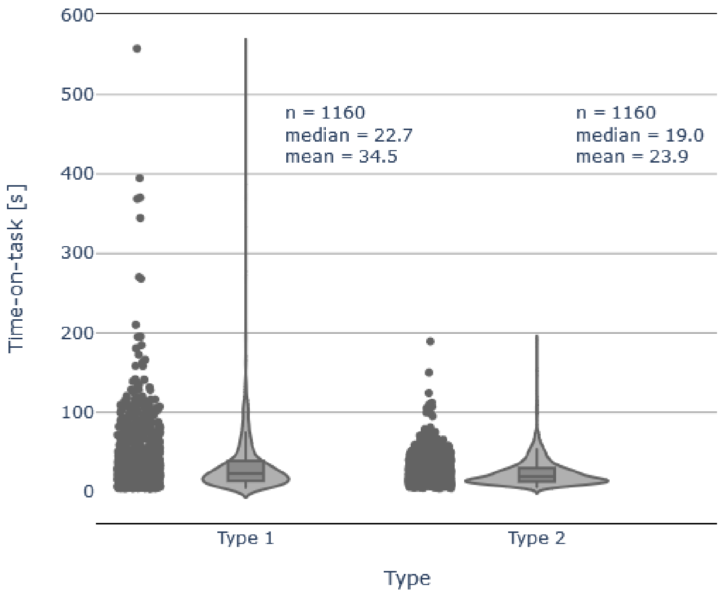
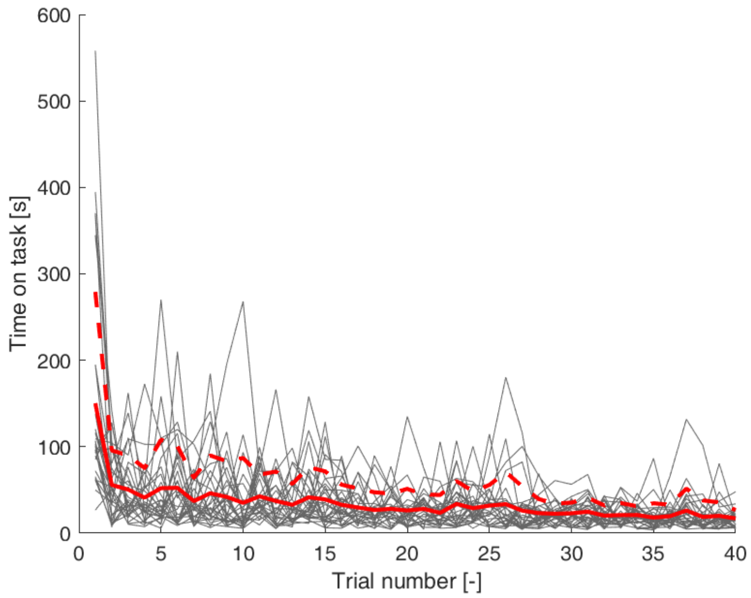


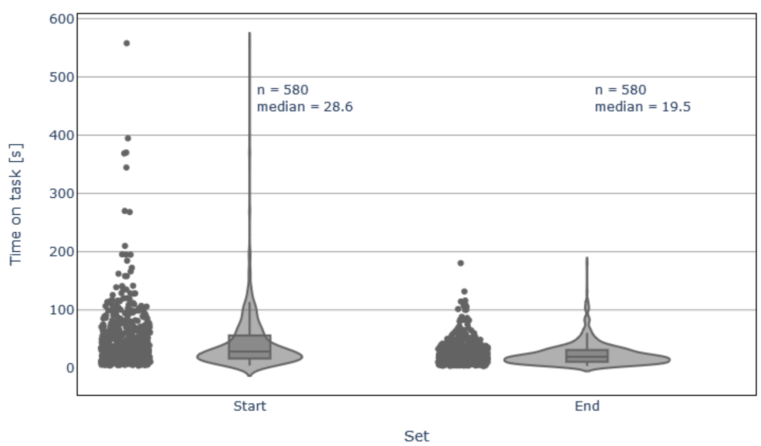
Figure 6.6: Time on task for type 1 and type 2 trials.

Learnability

The general usability of the interface depends on the learnability of the concepts and interactions necessary to operate the decision support system. This is especially true if the interface is used infrequently. Each of the experiments lasted for roughly one hour depending on the overall performance of the participant. The assumption prior to the experiments was that the users would perform slightly worse in the beginning of the experiment while getting more efficient over the course of the trials (see hypotheses H1 and H2). In order to check hypothesis H1, fig. 6.7a shows the development of the time on task over the trial number for each participant. One should note that each participant received the same set of questions, while the order of the questions was randomized for each experiment. The red solid line shows the average response time for each individual trial number. The red dashed line indicated the average value plus one standard deviation. The trend shows a steep decline over the first trials followed by a linear decrease afterwards. This indicates a high initial learning effect that remains less pronounced over the rest of the experiments. In order to test the significance of this improvement the Kruskal-Wallice test was performed by comparing the first 50% of the trials with the last 50% of the trials. The difference of the sets is significant according to the p-value of 1.59E-21, which is below the threshold of 0.05. Comparing both sets in fig 6.7b the median value dropped from 28.6s to 19.5s confirming the learning effect during type 1 trials that involved the manipulation of indicators.



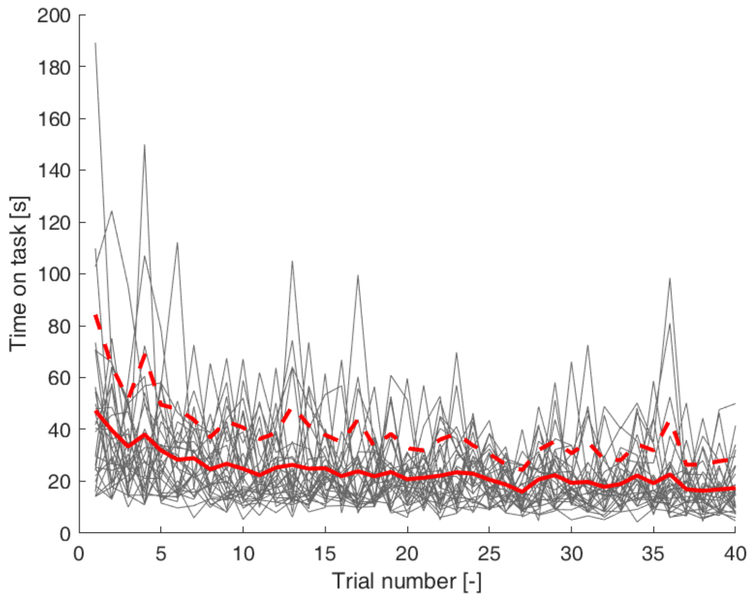
(a) Time on task over individual trial number for type 1 trials.



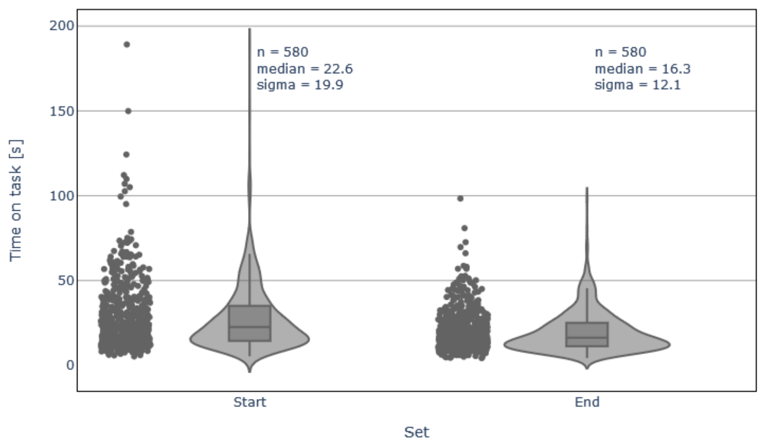
(b) Comparison of the starting and final set regarding time-on-task for type 1 trials.

Figure 6.7: Learning progression for type 1 trials, measured by time on task. The order of questions was randomized for each participant. The trial numbers refers to the individual sequence as perceived by the participant. Start/End p-value 1.59E-21

Fig. 6.8 shows the time on task for the 29 participants over the individual trial number for all trials of type 2. Here, the efficiency of insight generation was investigated. The average value is again depicted by a red solid line and exhibits a similar trend as in the case of type 1. However, the mean values are significantly lower than in case of type 1 (c.f. tab. 6.6 for p-values). Divided into two groups there is a significant difference in the starting and ending set with a change of median from 22.6s to 16.3s. Furthermore, the interquartile range is lower for type two trials, indicating a tighter distribution around the median value.



(a) Time-on-task over individual trial number for type 2 trials.



(b) Comparison of the starting and final set regarding time-on-task for type 2 trials.

Figure 6.8: Learning progression for type 2 trials, measured by time-on-task. The order of questions was randomized for each participant. The trial numbers refers to the individual sequence as perceived by the participant. Start/End p-value 1.67E-17

Table 6.6: p-values for the Kruskal-Wallis test to evaluate whether the differences between all groups are significant (< 0.05).

	Type 1 - Start	Type 1 - End	Type 2 - Start	Type 2 - End
Type 1 - Start		0.0000	0.0000	0.0000
Type 1 - End	0.0000		0.0000	0.0074
Type 2 - Start	0.0000	0.0000		0.0000
Type 2 - End	0.0000	0.0074	0.0000	

The compiled results prove a steep initial learning curve for both intended purposes. After an initial phase, the average response times further improve at a slower rate. This corresponds to well designed interface, whose functionalities and interpretation is intuitive to the average user. To confirm the interpretation of these objective results, the subjective user experience was recorded with a standardized SUS survey (cf. section 6.1.1). The SUS results are discussed below.

System Usability Scale (SUS)

The distribution of the SUS responses is shown in fig. 6.9 with median of 85.0 and a mean value of 81.2, at a standard deviation of $\sigma = 10.8$. According to Bangor et al. (2009) the average and median performance is rated excellent (see fig 6.1) and only one response is below the 63 threshold for acceptable performance. Fig. 6.10 further breaks down the subjective SUS scores to identify the areas where the DSS can be further improved. Exceptional scores were recorded for the topics complexity (2), others will learn quick (7), and the effort to learn (10). Thus, the subjective assessment of the learnalbility by the participants is congruent to the overall low response times and steep learning curve observed in the experiments. The other assessments average around a SUS score of 80, evaluating the performance between good and exceptional. The topics would use frequently (1), cumbersome (8) and confidence felt (9) are reflecting that the users did experience a small amount of frustration during the usage. Similar scores were achieved on the topics function integration (5), inconsistencies (6) and the needed amount of technical support (4), which give an indication on how the frustration was caused.

The distribution in fig. 6.9 is bimodal with the median values at 62 and 86, respectively. To investigate the cause for the grouping, the mean values for each questionnaire item are shown for both groups in fig. 6.11. There is no indication that specific categories are the cause for lower scores on in the blue category. The participants generally evaluated the decision support system on a lower level. Thus, the reason for the lower evaluation is likely to be found with the participant educational background or preparation.

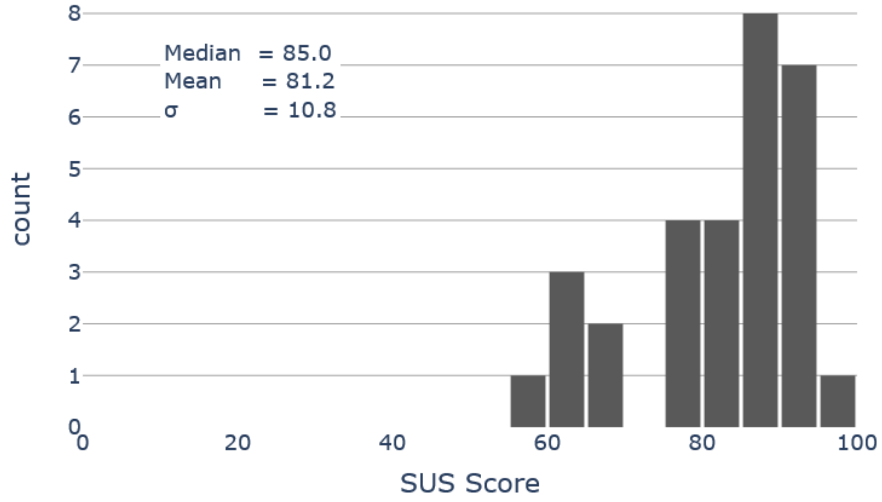


Figure 6.9: Histogram of the SUS scores for $n = 30$ participants.

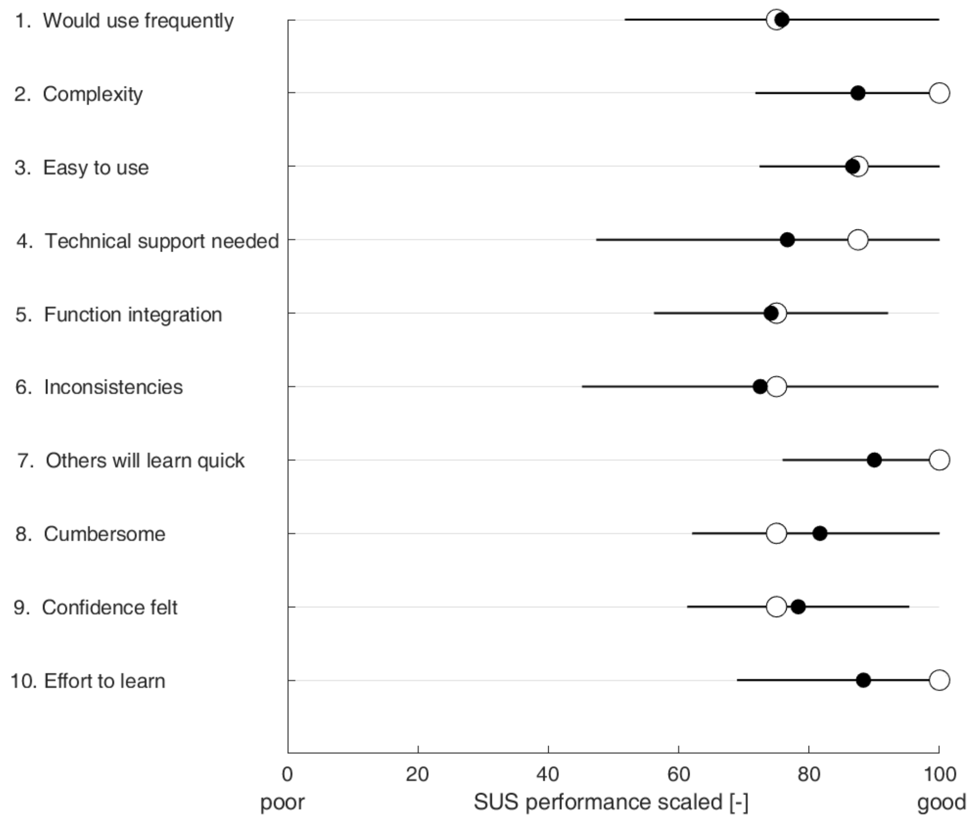


Figure 6.10: Scaled individual SUS scores for $n = 30$ participants. The mean (•) and median (◯) are indicated per question.

Figure 6.11: Mean values for all ten SUS questionnaire items. Color shows membership to the two bimodal groups.

6.3.2 Design concept evaluation (RQ B)

The design concept of the DSS is based on considerations of the SRK-framework and ecological interface design. By design, the trials targeted to assess the dashboard's performance with respect to insight generation and Pareto navigation by varying the difficulty levels. Evaluating the recorded performance metrics in relation to the difficulty level allows to screen for the correlation between the independent and dependent variables.

Efficiency of the selection interface

The efficiency of a decision support system can be measured directly by the time on task and the number of interactions required to arrive at the conclusion of the trial. An efficient design reduces the amount of interaction and interpretation, resulting in fast decision making with minimal possibilities to make mistakes. The time on task for each type 1 trial is plotted figure 6.12, grouped by category as described in section 6.2. The significance values for all combinations can be found in table 6.7 and are used to assess the experimental outcome regarding hypothesis H3.

Table 6.7: p-values of the Kruskal-Wallis test between all combinations of type one trials for the time on task. The p-value states the probability that the Null-hypothesis holds, which means that the combination of groups belongs to the same population.

	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
Type 1 - Cat 1		0.0000	0.0000
Type 1 - Cat 2	0.0000		0.0031
Type 1 - Cat 3	0.0000	0.0031	

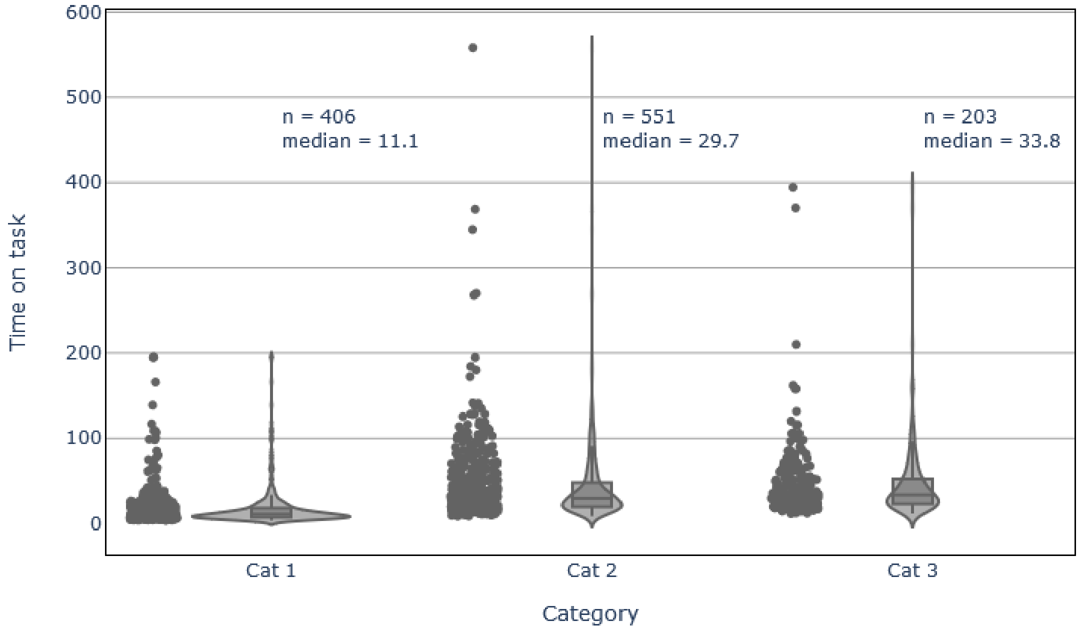


Figure 6.12: Time on task by category for type one trials, stated with their mean value and kernel density estimation. Category one: easy, category two: medium, category three: difficult.

The difficulty increases from category one to category three, with the number of active constraints on the indicators. As expected, the median response times are increasing with higher difficulty. The p-values listed in tab. 6.7 show that the null hypothesis can be rejected for all combinations of groups for a significance threshold of 0.05. Thus, the observed increase of median values is statistically significant. Category one trials are, on median, concluded after 11.1s with quartiles close to the median, which indicates a tight distribution (see fig. 6.12). In comparison, the time on task for category two trials nearly tripled at 29.7s with a twofold higher interquartile range (IQR). The median time on task for category three trials is 33.8s with a IQR comparable to the category two trials. The increase of the median is 13% and originates from two additional constraints and a slightly longer task text that need to be considered. Thus, the time on task does not scale linearly with the number of constraints for the first four constraints. The highest increase is observed during the transition from category one to category two trials, hence from one to two constraints on the solution. The single constraint case is almost trivial and thus easier to use.

The second dependent variable that is used to measure the differences in the efficiency of selection trials is the number of interactions needed to bring a trial to a conclusion. Figure 6.13 shows the absolute count of interactions that were recorded during all trials. The interactions are divided in three groups according to their difficulty level, with categories three, two and one from top to bottom. The interface elements from “benefit (BEN) up” up to “Not possible” are button interactions, followed by the tooltips hinting the indicator equations and the highlighting of traces and constraints in the time-series plots. For all categories the majority of interactions are in fact button interactions during the selection process. It is necessary to point out that it is not possible to draw conclusions from the absolute number of interactions within each category since the number of trials was not equal across the groups.

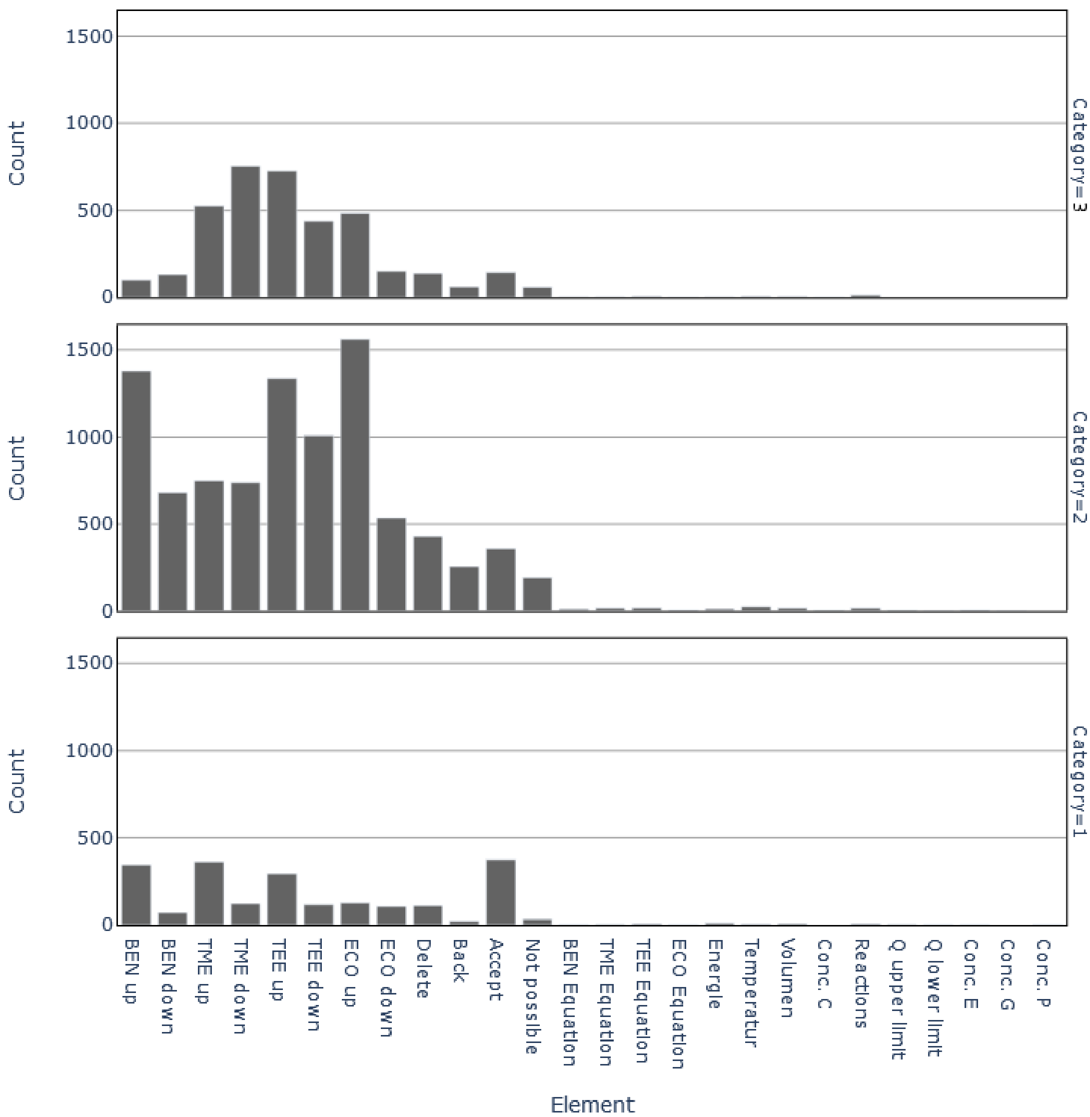


Figure 6.13: Count of interactions for all dashboard elements - type 1. Each row comprises the interactions for one category.

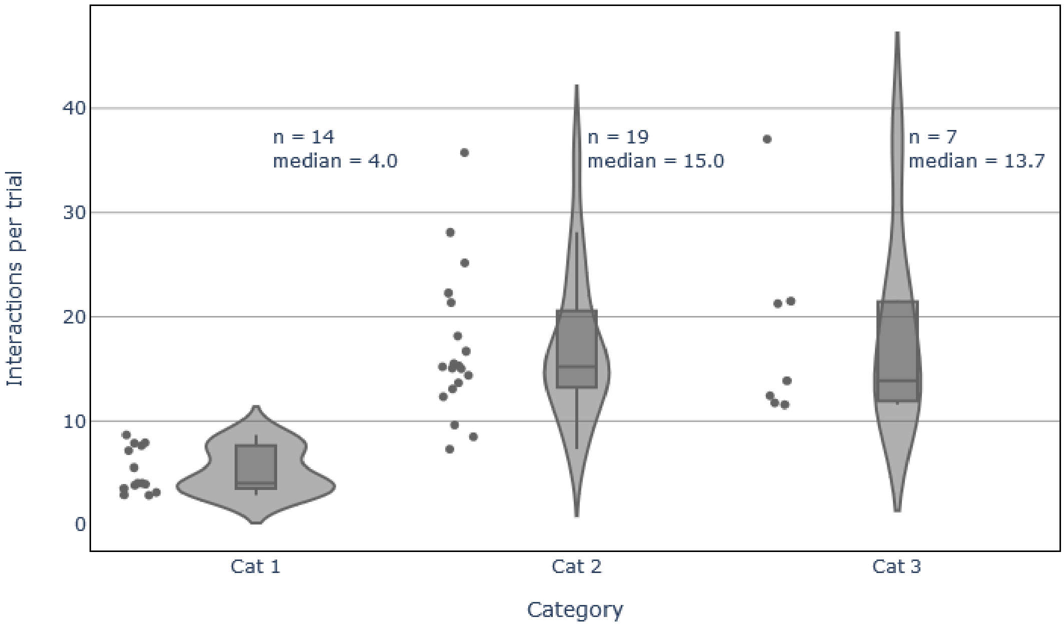


Figure 6.14: Overall interactions per trial by category - type one.

Hypothesis H4 aims to investigate if the task difficulty has a significant effect on the number of interactions per task. Fig. 6.14 shows the number of interactions per trial. Each point represents the average number of interactions via buttons, highlighting or the use of tooltips for one of the questions given to each participant. Analogous to the results observed for the time on task (c.f. fig. 6.12), category one trials exhibit a significantly lower number of interactions per trial compared to categories two and three. In contrast to the time on task the significance values in tab. 6.8 suggest that the groups of category two and three originate from the same population and do not exhibit significant differences.

Table 6.8: p-values of the Kruskal-Wallis tests between all combinations of type one trials for count of interactions per trial. Combinations where the null hypothesis H4 cannot be rejected are in **bold** print.

	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
Type 1 - Cat 1		0.0000	0.0003
Type 1 - Cat 2	0.0000		**0.8851**
Type 1 - Cat 3	0.0003	**0.8851**	

The median number of interactions per trial for category one is 4.0, which is close to the minimum of 2.0 interactions per trial. The minimum can be achieved if the correct "up" button is pressed and held down until the indicator is at it's maximum. The second necessary interaction is the button press accepting the selection. For category two and four the median number of interactions is 15.0 and 13.7, respectively. They are three to four times higher than in category one, which is consistent with the observations on the time on task. The fact that there is no significant difference between category two and three trials solidifies the deduction that the efficiency is more dependent on the classification according to the SRK framework than the number of constraints.

When looking at the number of interactions according to the types: button interactions, tooltip interactions and the use of highlighting within the time series plots (c.f. figs. 6.15a-6.15c), it becomes apparent again that the majority of interactions is affiliated to button interactions. The average interaction regarding highlighting and tooltips is below 0.4 per trial for all three categories. Whereas, the median number of button interactions is 4.0 for category one, 15.0 and 13.7 for category two and three respectively. Among highlighting interactions there is no significant difference between the category groups according to the results of the Kruskal-Wallis tests shown in tab. 6.9c. Concerning the tooltip interactions, a small but significantly higher level of interaction was recorded for category two and three in comparison to category one (see fig. 6.15b and tab. 6.9b). The same holds true for the button interactions, where the resulting p-values in 6.9a indicate that results for category two and three are not significantly different.

Table 6.9: p-values of the Kruskal-Wallis tests regarding hypothesis H4 for all types of interaction in interactions per trial. Only type one trials included by difficulty level. For p-values over 0.05 the null hypothesis cannot be rejected (**bold**).

(a) Button interactions.

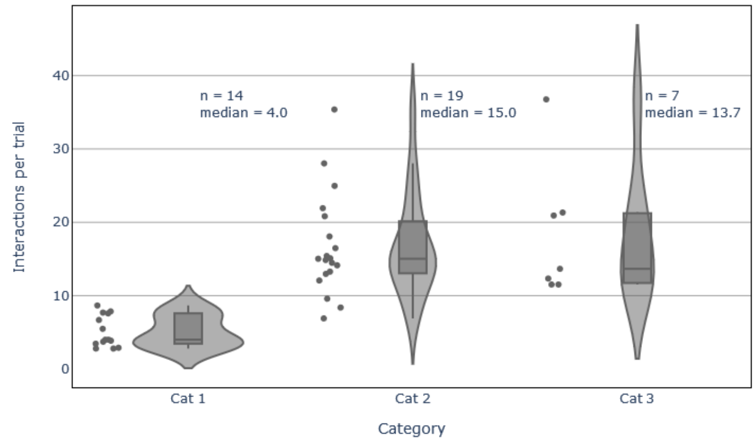
	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
T1 - C1		0.0000	0.0003
T1 - C2	0.0000		**0.9309**
T1 - C3	0.0003	**0.9309**	

(b) Tooltip interactions.

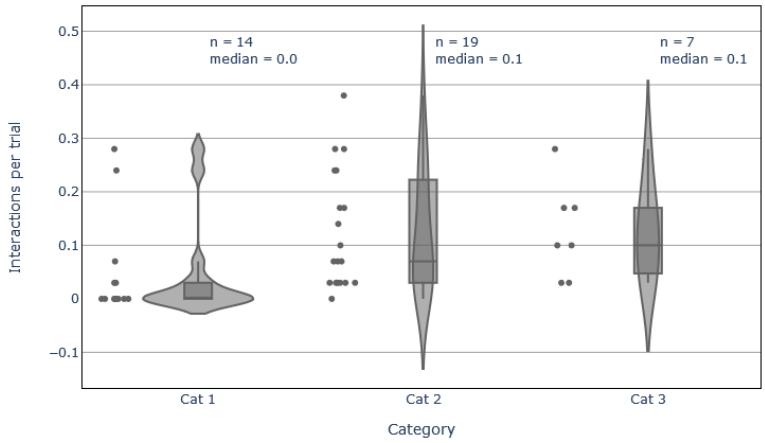
	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
T1 - C1		0.0029	0.0112
T1 - C2	0.0029		**0.7460**
T1 - C3	0.0112	**0.7460**	

(c) Highlighting interactions.

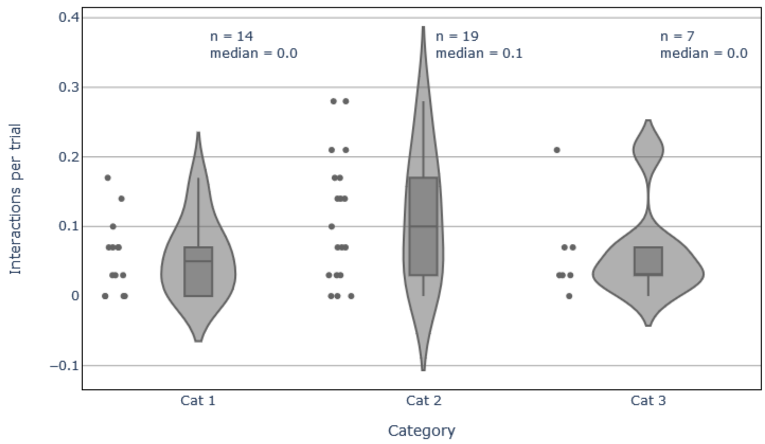
	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
T1 - C1		**0.0732**	**0.9082**
T1 - C2	**0.0732**		**0.2299**
T1 - C3	**0.9082**	**0.2299**	



(a) Button interactions per trial by category - type 1.



(b) Tooltip interactions per trial by category - type 1.



(c) Highlight interactions per trial by category - type 1.

Figure 6.15: Interactions per trial by category for type 1 trials.

Effectiveness of the Pareto navigation

Generally, the effectiveness of a task is evaluated by the proportion of correct answers compared to errors. For type 1 tasks a result was registered as correct if an operating point was selected that satisfied all requirements stated in the task. The selection was achieved via interaction with the buttons below the bullet charts as shown in fig. 5.23 and acknowledging the final selection by pressing the "accept" ("Akzeptieren") button. In cases where the requirements could not be fulfilled the user needed to press the "goal not possible" ("Ziel nicht möglich") button on the lower left corner (c.f. fig. 5.22). It was not possible to skip any tasks, thus the share of correct and incorrect trials adds up to 100%. Figure 6.16 shows the share of correct and wrong trials per category for a total of 1160 trials. Note that the distinguished categories are one, two and three, with an increased number of constraints imposed on the selected operating point. Quite surprisingly, the highest failure rate is observed for category two with as much as 20% errors. This is consistent with the higher number of interactions per trial for category two trials, as shown in fig. 6.13, fig. 6.14 and fig. 6.15. For category one and three the recorded error rate was 7.9% and 6.9%, respectively. Figure 6.17 shows the error rates for trials where the

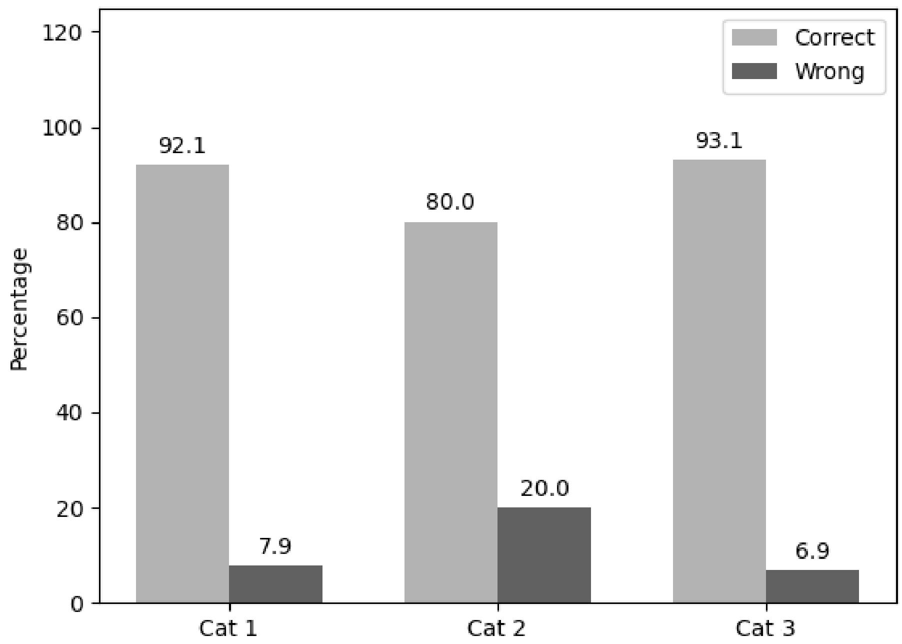


Figure 6.16: Statistics on the accuracy of the decisions made by category for trials of type 1 for a total of 1160 trials.

target performance could not be achieved. One can see that the failure rates for impossible tasks were lower in all categories, implicating that the trials were easier to solve correctly.

Fig. 6.18 displays the error rates per type one question, grouped by category. In conjunction with tab. 6.10, hypothesis H5 can only be rejected for the comparison of categories one and two. For all other combinations of test groups there is no statistically significant difference for a p-value threshold of 0.05 according to the Kruskal-Wallis test.

The observed error rates per question in category two have some outliers with $45 - 78\%$. Further investigation revealed that the corresponding questions are of a similar type: they require one of the indicators to be set to a specific value and subsequently the maximization of another REI. The reason for the increased error rates could not be deduced from the recorded experimental data, but multiple scenarios are possible: (1) these questions are statistical outliers, (2) the users adjusted the wrong indicators due to insufficient labeling, (3) they misunderstood the question or (4) they manipulated the indicators in the wrong order, starting with the maximization and being not able achieve the requested value. Option (2) remains unlikely, since the labeling is the same in all trials. Alternatives (3) and (4) result from an error in the identification of the targets. Additional experiments are necessary to determine if the design needs to be improved to reduce outliers (1 or 2) or if the experimental design was flawed (3 or 4). The latter case would not require changes in the design, since this source of error is eliminated in real application cases. The target is a managerial decision by the user and cannot be

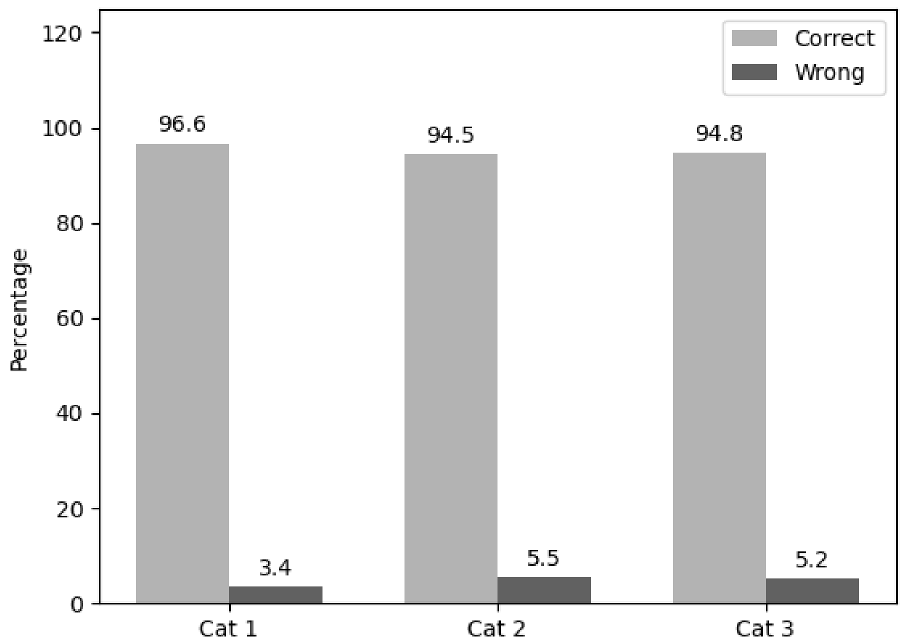


Figure 6.17: Statistics on the accuracy of the responses in case the objective was not achievable.

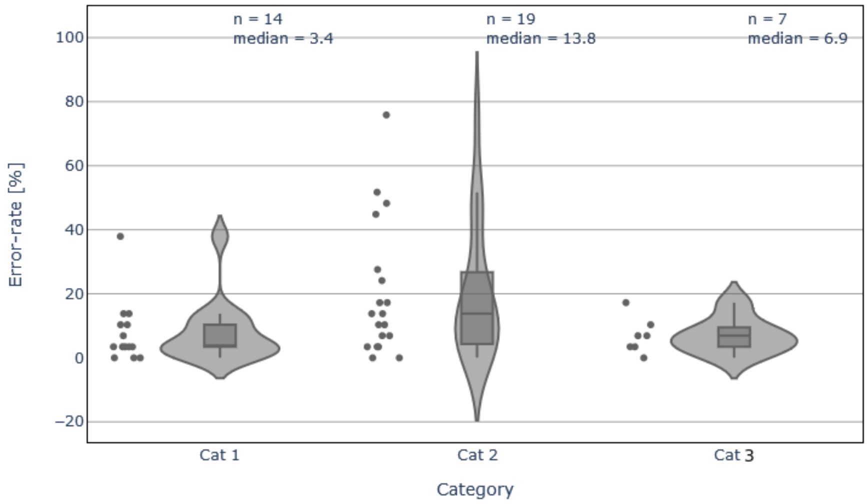


Figure 6.18: Error rates in % of type one trials by difficulty level.

misunderstood, because no communication takes place.

Table 6.10: p-values of the Kruskal-Wallis tests obtained for the error rate per questions for all combinations categories. Only the differences between category one and two are statistically significant. For p-values over 0.05 the null hypothesis cannot be rejected (**bold**).

	Type 1 - Cat 1	Type 1 - Cat 2	Type 1 - Cat 3
Type 1 - Cat 1		0.0410	**0.7889**
Type 1 - Cat 2	0.0410		**0.1228**
Type 1 - Cat 3	**0.7889**	**0.1228**	

Efficiency of insight generation

Type 2 trials aim to evaluate the ability of the interface to elucidate the causal chain from operational inputs over the system trajectories to the resulting efficiency indicators. Again, the response times are evaluated in three groups: in category one the user needed to identify the changes in the efficiency of one REI between the previous and current operating point. Category two trials aim to evaluate the understanding of the movement made on the Pareto frontier and the corresponding trade-offs. Category three trials included reasoning of the cause and effect relationships alongside the causal chain from inputs over the dynamic batch trajectories to the impact on REIs.

Figure 6.19 shows the distribution of the time on task for trials of type 2. With increasing task difficulty the median value and IQR increase, because the user must evaluate more

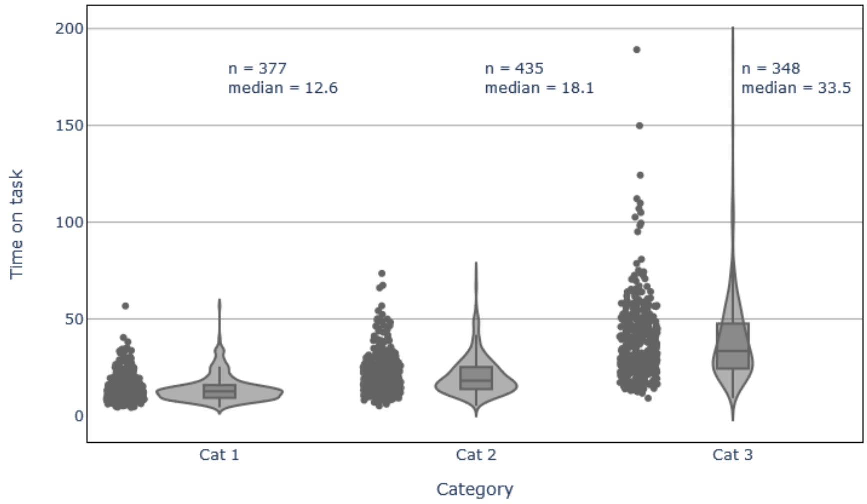


Figure 6.19: Time on task by category for type 2 trials. The distribution is skew towards zero.

Table 6.11: p-values of the Kruskal-Wallis tests between all combinations of type two trials for the time on task. The p-value states the probability that the hypothesis H6 holds, hence that the combination of groups belongs to the same population. The null hypothesis can be rejected for all combinations (¡0.05).

	Type 2 - Cat 1	Type 2 - Cat 2	Type 2 - Cat 3
Type 2 - Cat 1		0.0000	0.0000
Type 2 - Cat 2	0.0000		0.0000
Type 2 - Cat 3	0.0000	0.0000	

causal relationships. This directly translates to an increased time on task, where the median value grows from from $12.6s$, over $18.1s$, to $33.5s$ for category three trials. At the same time the IQR grows from $6.52s$, over $11.4s$, to $23.2s$, indicating that the distribution spreads further for higher difficulties. The p-values listed in tab. 6.11 validate the findings as statistically significant according to hypothesis H6, since the probability that any of the groups originate from the same population is close to zero.

The second measure to evaluate the efficiency of insight generation is the number of interactions necessary to validate or disprove the statements in type two trials. Since type two trials only involve exactly one button interaction ("OK"), highlighting and tooltips are the only interactions that are relevant to be examined. Figure 6.20 shows the absolute count of interactions recorded for each category. Across all categories, the reactions tooltip was used frequently. It is situated next to the reactor sketch and

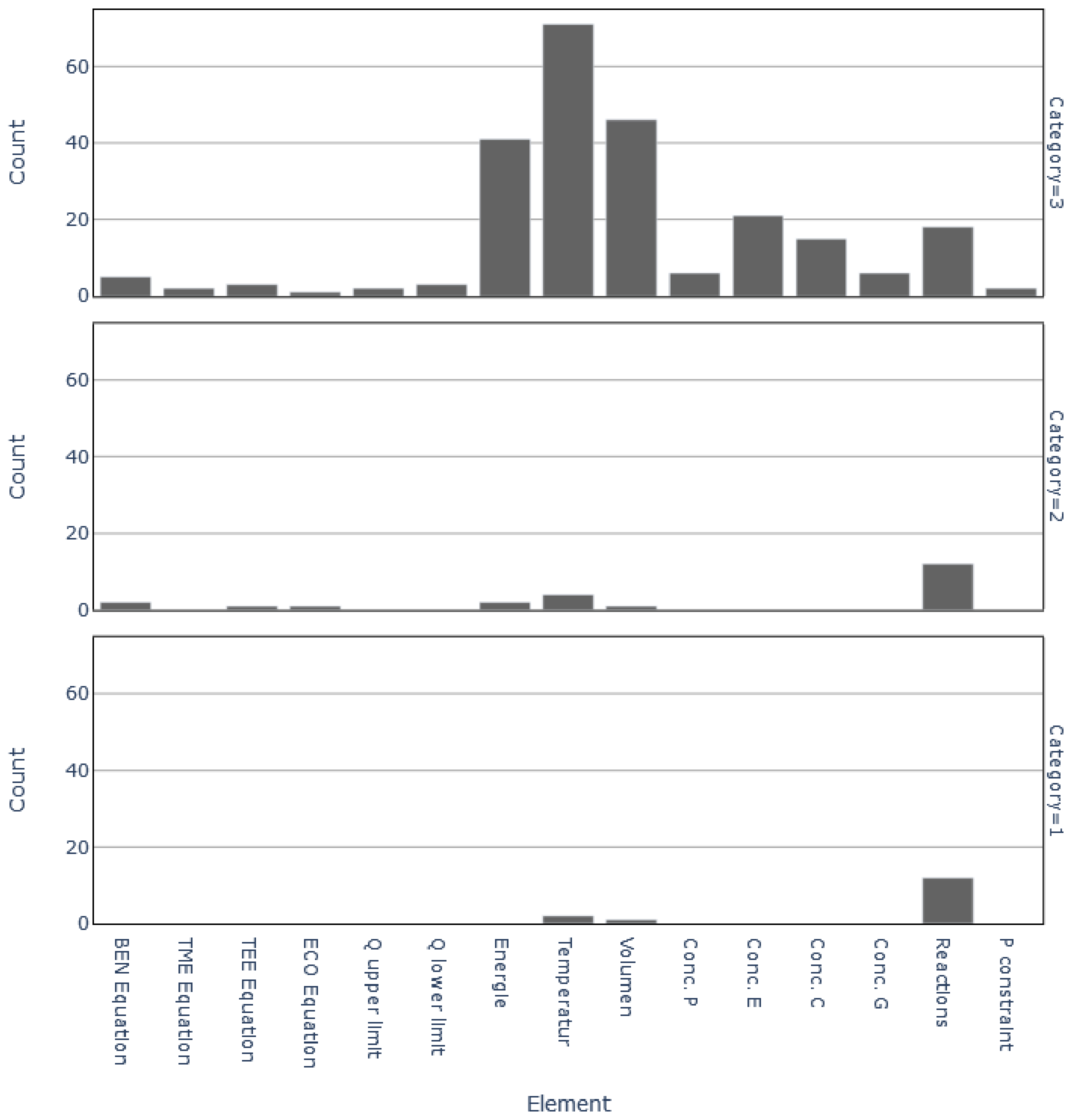


Figure 6.20: Count of interactions for all dashboard elements - type 2. Each row comprises the interactions for one category.

displays all reaction equations. For category one the only other observed interactions are the highlighting functionality for the volume and temperature trajectory. Observing any interaction for category one trials is unexpected, since the entire information needed for the assessment is shown in the bullet charts. The same type of aid is observed for category two trials, with a low amount of additional request for indicator definitions. Since category two trials include the assessment of the movement of indicators relative to each other, the same information from the bullet charts representation is needed, with the exception that now multiple indicators are relevant. Thus, the absolute count of interactions for categories one and two are small when compared to category three. Here, the main interaction is, as expected, highlighting batch trajectories for the reactor temperature, the volume, and concentrations. The highlighting procedure is useful to distinguish the trajectories before and after the change, which is necessary to test the reasoning process of all three possible responses to the task.

Table 6.12: p-values of the Kruskal–Wallis tests between all combinations of type 2 trials for count of interactions per trial. The p-value states the probability that the Null-hypothesis holds, hence that the combination of groups belongs to the same population. For p-values over 0.05 the null hypothesis cannot be rejected (**bold**).

	Type 2 - Cat 1	Type 2 - Cat 2	Type 2 - Cat 3
Type 2 - Cat 1		**0.4040**	0.0000
Type 2 - Cat 2	**0.4040**		0.0000
Type 2 - Cat 3	0.0000	0.0000	

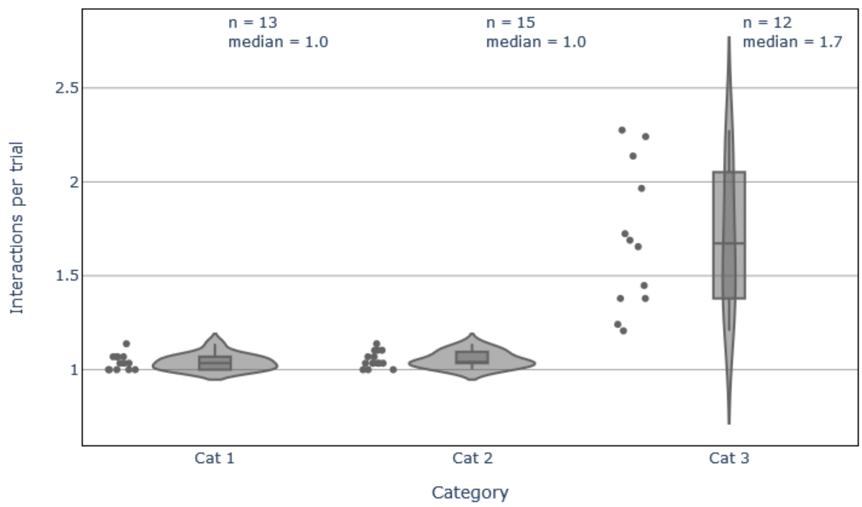


Figure 6.21: Overall interactions per trial by category - type 2.

To substantiate the observations from fig. 6.20, the hypothesis H7 was evaluated for the number of interactions per trial and summarized in fig. 6.21. The medians for category one and two are at the theoretical minimum, because at least one interaction is necessary to acknowledge the selection by pressing “OK”. According to table 6.12, only category three exhibits a significant increase in the interactions per trial, with an median value of 1.7 interactions per trial at a standard deviation of 0.4. These results are in line with the assessment of the absolute count of interactions in fig. 6.20

Effectiveness of the insight generation

Analog to the effectiveness of the selection interface, the error rate during type two trials is used to assess the effectiveness of the interface with respect to insight generation. Figure 6.22 displays the percentage of correct and wrong responses per category. Compared to type 1 questions the error rates are lower, but also exhibit a slight increase for higher difficulty levels with 0.8% for category one, 1.6% in case of category two, and 4.0% for category three. Higher categories involve more information that needs to be validated to make a decision. Hence, the probability for misinterpretation increases as well.

Hypothesis H8 evaluates if changes in the difficulty level cause an impact on the error rates per trial. Fig. 6.23 shows the distributions of error rates per type 2 trial. The corresponding Kruskal–Wallis results in tab. 6.13 indicate that all p-values are above 0.05 for all combinations of groups. Thus, the Kruskal–Wallis test could not reject the possibility that all the samples originate from the same population and differences in the median values and IQR are purely coincidental. The median values are zero for categories one and two, with a non-significant increase to 2.2% in category three. The insight generation created by the decision support interface results in low error rates during the assessment of the inner relations between inputs, system dynamics and the resulting resource efficiency.

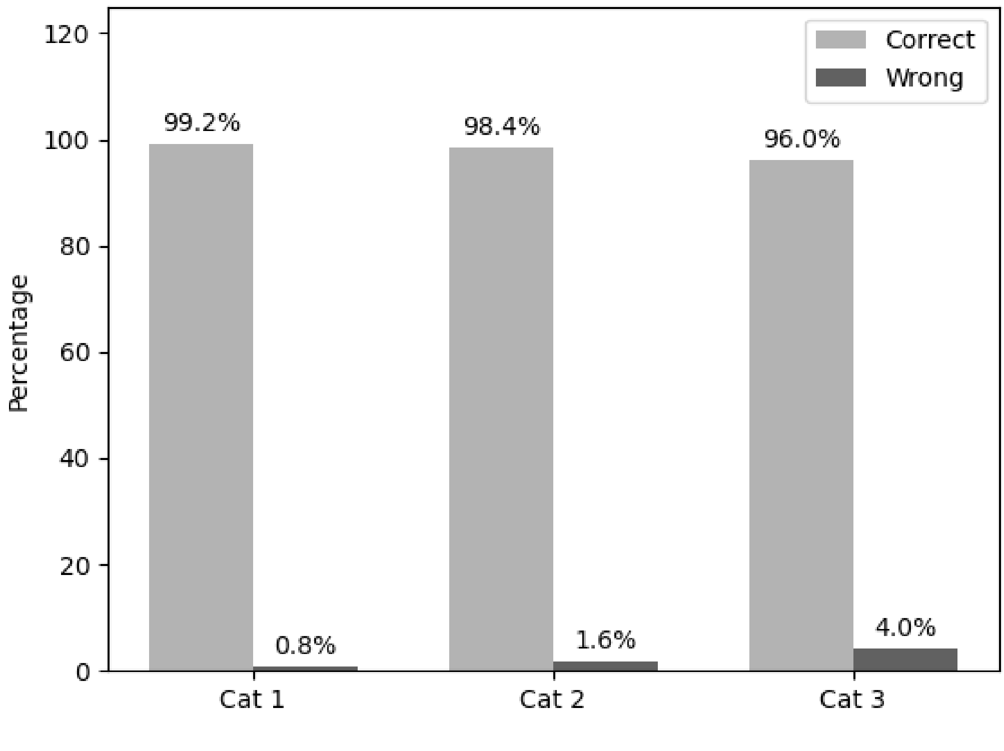


Figure 6.22: Statistics on the accuracy of the decisions made by category for trials of type 2 for a total of 1160 trials.

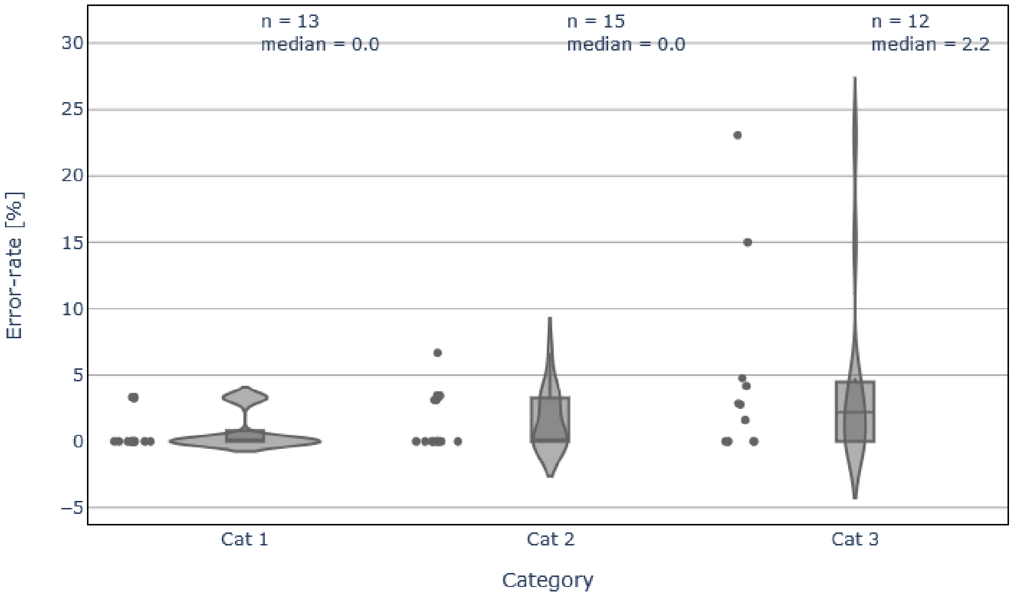


Figure 6.23: Error rates in % of type two trials by difficulty level $1 - 3$.

Table 6.13: p-values of the Kruskal–Wallis tests between all combinations of type 2 trials for error rates per trial. The p-value states the probability that H8 holds. For p-values over 0.05 the null hypothesis cannot be rejected (**bold**).

	Type 2 - Cat 1	Type 2 - Cat 2	Type 2 - Cat 3
Type 2 - Cat 1		**0.3036**	**0.0749**
Type 2 - Cat 2	**0.3036**		**0.3573**
Type 2 - Cat 3	**0.0749**	**0.3573**	

6.4 Discussion

In Chapter 4 an adaptation of the Williams-Otto semi batch reactor was used as an application case to show how the resource efficiency and economic performance can be captured in REIs. A multi-dimensional optimization problem with four REIs was defined and solved to obtain the set of Pareto–optimal solutions by control vector parameterization in combination with the normalized normal constraint method. Based on the results, a decision support system was developed that followed the considerations of design methodology in section 5.3. Specifically, the interface should support the navigation on the Pareto-frontier and an optional insight generation to intensify the process understanding. It was assembled from visualization elements specifically screened for their suitability in the scope of resource efficiency optimization (see section 5.2). The design process followed the ecological interface design framework (section 5.1.2) and involved expert interviews to arrive at the final design, outlined in section 5.4.3.

The final design was implemented in MATLAB® and evaluated by the usability study reported in this chapter, regarding the three indicators: efficiency, effectiveness, and user satisfaction. Furthermore, the difficulty levels were varied for both functionalities to conduct a design concept evaluation that assesses if the assumptions made during the ecological interface design process are in line with expectations according to the skill-, rule-, and knowledge-framework.

6.4.1 Usability evaluation (RQ A)

The **efficiency** of the DSS was evaluated by the recorded time on task until the user arrived at a decision. The main objective of the DSS is to aide in the selection process of a new operating point among Pareto-optimal alternatives. Here, the user experiences the system inherent trade-offs between the REIs and is able to investigate if the desired performance is in fact possible. The secondary objective is to explain to the user how the requested efficiency can be realized by supplying the necessary input values and the supporting information about the system dynamics that ensue and result in the REIs. Prior to the experiments the time frame of $5min$ was given as a target performance for the complete decision making process. This includes the selection process and the process of understanding how the proposed inputs are causing the desired indicator values. Both objectives were investigated separately by type 1 and type 2 trials. In total only 1.5% of the type 1 and 0.08% of the type 2 trials exceeded a time on task of 2.5min that was awarded to each objective. The observed median response times were $22.7s$ and $19.0s$, respectively. Thus, the DSS design meets the efficiency target.

The second factor for the usability of a system is the **effectiveness** with which a user achieves a specified goal during use. A high effectiveness is obtained when the goal is reached correctly and completely. The main task of the system is to select a suitable operating point with the desired performance in terms of resource efficiency (function 1). In the experiments this was simulated by type 1 tasks, where the participants were correct in 87% of the cases with their selection. The secondary task, explaining system relationships, was solved with a much lower error rate of 2%. The difference in the observed error rates is probably due to the fact that the user was given three answer options for type 2 tasks that can be validated by the information presented. Additionally, the Pareto navigation tasks require an active use of the interface to select an operating point, which in turn increases the probability of making mistakes. The target of a maximum error rate of 10% was narrowly missed in the case of type 1 questions with

13%, while questions concerning understanding trials were answered very accurately. The relatively high error rate in case of the main function is unfavorable, since it can lead to the selection of operating points that do not correspond to the goals. However, the proposed operating points are always on the Pareto Front and are therefore still optimal with respect ot the multi-objective optimization problem.

The third and last factor of usability of a system according to ISO9241-11 is the **satisfaction** of the user during usage. In contrast to the factors already evaluated, it is not easy to measure user satisfaction by objective measures. The ISO9241-11 standard lists the learnability of systems as a key factor for user satisfaction. The experimental results show a steep learning curve at the beginning of each experiment, which continues at a reduced level over the remaining experiments and is at a statistically significant level. In addition to the objectively measurable variables, a **SUS questionnaire** was distributed to all participants after the experiments to reflect subjective impressions. With a median score of 85.0 and an average of 81.2 on the System Usability Scale the DSS shows an excellent result according to Bangor et al. (2009). The results of the SUS survey prove the good usability of the DSS system and support the predominantly positive results regarding efficiency, effectiveness and learnability.

6.4.2 Design concept evaluation (RQ B)

The design of the decision support systems aims to reduce the cognitive load experienced by the user. In general, it is expected that an increase in task complexity reduces the effectiveness and efficiency of the system. The design process aims to preprocess the information to the extent that the user can intuitively deduce the relevant conclusions. Within the SRK-framework, such activities are referred to as skill-based behavior and describe the simplest form of processing. If the user has to weigh several pieces of information against each other by means of rules, this is called rule-based behavior. Here, the expected error rate increases. As soon as the user has to bring his experience with the system into the interpretation, it is called knowledge-based behavior, which is the most demanding form of decision making. In order to test the anticipated influences of the difficulty levels on the performance variables, the type 1 and type 2 tasks were divided into three difficulty levels each, as described in Section 6.2.2. The Kruskal-Wallis test can be used to test the hypotheses formulated in Section 6.2.2 and determine if the level of difficulty is consistent with the expectations according to the SRK-framework.

Efficiency of the navigation interface
The experimental results by level of difficulty indicate a significant increase for the time on task from category one to category two. The additional increase to category three is smaller, however significant according to the Kruskal-Wallis test. Part of the increase can

be attributed to longer task texts, since it is necessary to describe additional constraints. However, the largest part of the increase is likely due to the step from skill-based behavior to rule-based behavior with the corresponding increase in cognitive load (c.f. section 5.1.1). In case of category one trials only one indicator needs to be manipulated. For 86% of tasks one of the indicators needs to be maximized by pressing and holding the up button for the corresponding indicator. For category two trials, two indicators must considered and referenced against each other. It might be necessary to reiterate the selection between both KPIs because a selection of one indicator can significantly reduce the possible range on the other. This amount of rule-based interaction explains the observed increase in the observed time on task. The additional increase in category three trials is most likely due to the additional constraints that need to be considered. However, even though the amount of constraints doubled from two to four, the time on task only increased by 13%, opposed to the growth of 168% between the first two categories. It is plausible to assume that the progression from skill-based to rule-based behavior is impacting the performance more severely than the number of relevant constraints in solving Pareto navigation trials. Thus the design of the DSS is highly scalable for multi-criteria optimization scenarios.

On further inspection, for all categories the majority of interactions are in fact button interactions during the selection process. Since tooltips and highlighting interactions were only regarded as supporting information, this picture is indicative of a good design with respect to the decisions made on what information to display continuously and what to supply by optional elements. A design flaw would be apparent if any of the optional data would have been requested more often.

The efficiency of the investigated selection interface is sufficiently good, since the median time on task was below 35s for all difficulty levels. Furthermore, there are hardly any outliers above two minutes, which is still considered to be sufficiently fast, because the on-site use of the decision support system is not time critical and the achieved values seem reasonable. The evaluation of hypothesis H4 revealed that the number of interactions per trial was significantly lower for category one trials, while H4 could not be rejected in the comparison of categories two and three. This further supports the notion that the deterioration in performance can largely attributed to the shift from skill- to rule-based decision making.

Effectiveness of the navigation interface

The overall effectiveness of the selection interface is satisfactory for categories one and three with error rates below 8%. Furthermore, operational points that cannot be achieved are identified reliably by the user for all categories (see 6.17). However, there remains potential for improvement in category two trials. The increased error rate of 20% is due to a small number of outliers that reduce the overall accuracy of decisions and need to be further investigated. Possible reasons for an error can be:

- Falsely assessing an achievable objective as impossible,
- evaluating an operating point as compliant with the constraints imposed by the task, while it is not,
- ambiguously worded tasks,
- or a share of the participants was guessing.

The first case would arises if the user does not exploit the possibility to reiterate his or her previous decisions to the fullest extent. Furthermore, the first two cases can arise if the indicators are mistaken for each other and the user is under the impression that the goals are achieved, while they are achieved for the wrong combination of indicators. The error rate for some of the category two tasks was higher than 50% suggesting that ambiguously worded tasks might have played a role. It would be worthwhile to design another experiment aiming to investigate this further, since it is highly desirable to reduce the error rate towards a greater impact on resource efficiency.

Despite the identified drawbacks, the current version of the interface is able to deliver valuable decision support. The vast majority of evaluated cases led to the selection of an desired operating point, thus contributing to the resource efficiency of the system.

Efficiency of the insight generation
Overall, the efficiency aligns with the expectations. The time on task is increasing with the number of steps in the causal chain. The time on task is observed to be maximal in category three trials with a median $33.5s$, with the upper 75%-percentile below $50s$. This appears to be a reasonable time frame, when keeping in mind that the evaluation is only warranted during the initial phase of decision support. Within this scope the user is sufficiently fast and can back-trace the reasoning behind the selected efficiency as desired. The analysis of interactions revealed that the information directly supplied by the interface, without the need of optional highlighting, is sufficient to understand the changes in the efficiency of a single indicator (category one) and the rule-based assessment of trade-offs between multiple indicators. The user only depends on the optional information in the form of tooltipps, if inner system relations between inputs to REIs is investigated. This attests to a balanced dashboard design that does not overload the user during ordinary decision support tasks, while having additional information ready if requested to improve the level of acceptance.

Effectiveness of the insight generation
The experimental results for type two trials indicate a high accuracy in the recognition of cause and effect relationships, as well as in the identification of trade-offs and hence in the exploration of the Pareto frontier. The increase in error rates observed for more difficult

trials is below the significance threshold and less than 4% absolute. This performance is better compared to the effectiveness of the selection interface and regarded as highly suitable for the intended purpose.

6.5 Conclusions

The decision support system developed in Section 5.4 supports the user in the selection of an operating point on the Pareto-front and enables the user to understand the system interrelationships leading to it. The design of the DSS was developed based on the SRK framework and the Ecological interface design (EID). The goal of the EID concept is to reduce the cognitive load of the user by preparing the necessary information in a way that it is easy to consume and if possible already in aggregated form. In general, a reduction of the cognitive effort can also shorten the necessary time on task and reduce the error rate, which is both desirable for effective decision support. In addition to efficiency (time on task) and effectiveness (error rate), good systems are characterized by high user satisfaction.

The participants of the study were recruited among engineering students, as they are similar to the intended user group through their education. However, they differ in the level of system knowledge from users in industry, as they are not familiar with the considered reaction system prior to the experiments. At this point, it is assumed that a decision support system that meets the desired performance criteria for inexperienced users will also lead to success for the intended users among the plant management. This assumption should be tested in an industrial setting.

The study in this chapter examined the result of the design process regarding the subjectively perceived and objectively measured usability, on the basis of a standardized questionnaire, as well as the ISO9241-11 criteria efficiency, effectiveness and user satisfaction. A systematic distinction was made between the functions of navigation on the Pareto-Front and the explanation of the system interactions. The subjective impression of the test subjects after using the system for approximately one hour is expressed by an average and median value for the SUS score of 81.2 and 85 respectively. According to Bangor et al. (2009), such a result can be classified as excellent and thus indicates a high quality of the DSS. The subjective evaluation is supported by reaction times well below the target value of 5 minutes and a steep learning curve at the beginning of the experiments. The learning effect was evaluated by comparing the response time for the first half of all trials with the second. The error rate of 13% for Pareto navigation tasks is slightly above the target value of 10%. A closer examination of the results reveals that the relatively high error rate is caused by four outliers in the type 1 questions. The questions are characterized by a similar phrasing of the question, which could be the cause of the outliers. Further experimental investigations could determine whether the type or phrasing of question has an influence on the error rate, but were not conducted withing the scope of this thesis. If so, this effect would be irrelevant for the performance of the system, because the objective in real life does not result from a formulated statement but from a managerial decision of the user.

The additional subdivision of the tasks for both functionalities according to their difficulty enabled to verify the basic assumptions of the SRK-framework. Regarding the efficiency of the system, the results follow the expected effects. The largest increases in time on task are observed at changes from skill-based to rule-based, or further to knowledge-based decision making. The effectiveness, measured in terms of error rates per question, is not significantly dependent on the difficulty of the task and is low. The only deterioration in the error rate is due to the above mentioned outliers in category two of type one. The nature and scope of the decision support suggests a use in two scenarios. The first is shortly after the introduction of the system, as management is dealing for the first time with the issue of multi-dimensional resource efficiency, and the second is each time the targets shift between the competing indicators. Thus, the DSS is used relatively infrequently and it is possible that prior learnings are forgotten. Therefore, it is even more important that users can quickly re-learn how to use the system and that the system is designed to be as intuitive as possible. The experiments could show that even the first interactions with the system could be solved within the given target for the processing time. Thus, a sufficiently intuitive design can be assumed and the conducted study was able to confirm a high quality of the decision support system, as well as the underlying assumptions of the SRK-framework.

Chapter 7

Overall conclusions and outlook

In this thesis real-time REI were defined that are able to capture the resource efficiency of batch processes. First, a framework was developed in Chapter 3 that can be used to describe the local efficiencies for each unit operation. Using a vertical aggregation approach, a mean plant efficiency can be obtained. Alternatively, the local efficiency contributions can be propagated along the process to assess each batch separately on unit and plant level. The propagation approach was successfully implemented in the application case of a sugar plant to optimize the operational degrees of freedom towards a global optimum (Chapter 3.5). The application case optimized the energy efficiency of a hybrid plant that combines batch-wise and continuously operated production units.

The sugar plant application cases implemented a decision support solution with a one dimensional resource efficiency objective. Chapter 4 extends the approach to the multi-dimensional case, with a total of four objectives: energy efficiency, material efficiency, eco-performance and the economic benefit. The solution of multi-objective optimization problems is a set of Pareto-optimal operating points that reflects a trade-off between the individual optima. Here, decision support translates to the navigation on the Pareto frontier, according to the managerial preferences of the decision maker. The output of the DSS is the set of process inputs that lead to the requested efficiency metrics. Thus, a process model must be available that is able to predict the variables relevant to the REI. In Section 4.2 a first principle model describes the process dynamics of the Williams-Otto semi-batch reactor, while the NNC algorithm is used to sample the Pareto front. The efficiency of each point is recorded with the associated set of inputs in order to enable decision support.

In Chapter 5 available visualization elements were screened for their suitability to display resource efficiency related information for batch and batch-continuous production processes. Based on SRK- and the EID-framework, a methodology was developed to compose efficient and effective decision support to deliver two core functionalities: the selection process of a desired operating point, and the generation of insights into how the desired resource efficiency metrics can be achieved in the multi-dimensional case. The design is a result of considerations to minimize the mental load during the decision making process targeting a low error rate and an efficient, decisive interaction. The key is to preprocess the available information and to assemble a concise dashboard that contains only the relevant data. A secondary set of information was identified that is useful for a root cause analysis and provided additionally as tooltips and highlighting information. The methodology was applied to the WOSBR example introduced before, as described in Section 5.4.

Finally, in Chapter 6 the usability of the DSS was assessed with an experimental study to reference objective measures for efficiency and effectiveness against the subjective impression of the study subjects. The assessment was conducted for two particular intentions: the efficient navigation on the set of Pareto optimal solutions and the optional target of insight generation. The results indicate that the differentiation between primary and secondary information was correct, since secondary information was rarely requested during the navigation process. The insight generation for the first step in the root cause analysis was also possible without secondary information. Only the reconstruction of the entire chain of reasoning from inputs, over dynamic behavior, to the resulting efficiency indicators required an occasional usage of supporting information. This DSS functionality is optional and only targets the introduction phase to increase the users trust in the results of the DSS. The efficiency of both functionalities was measured via the time on task for trials of varying difficulty and was consistent to expected cognitive load. The effectiveness, measured by the error rate, was excellent for insight generation tasks on all difficulty levels. However, there was a 20% error rate recorded for selection trials of medium difficulty that was significantly higher than trials from the categories “easy” and “difficult”. The cause of this deficiency could not be identified in this experiment, but it was possible to derive theories that can be investigated in further experiments. Nevertheless, the high error rate of 20% is not crucial for the operation of the process, since a mistaken selection is still within the Pareto set.

This thesis contributes a methodical approach to deliver decision support to optimize the resource efficiency of batch production processes. The method was successfully used to optimize an industrial process in an iterative real-time scheme, in the global optimization of a hybrid production process and a model-based Pareto navigation case. In the development of decision support solutions, this thesis focused on cases where a model of the production process was available. In cases where no model is available data driven methods need to be used. Beisheim et al. (2019, 2020) reported the REIs and a data-driven model for the best-demonstrated practice (BDP). The BDP is a function of the external influences and is hence adjusted for non-influenceable factors. The difference between these two values is seen as operator improvement potential (OIP) and reflects the optimization potential, which can be obtained by optimal inputs under the current circumstances. To further improve the methodology developed in this thesis, the baseline for each production unit could be obtained analogously to the publication Beisheim et al. (2019) and subsequently propagated, according to the methodology in Chapter 3, to assess the improvement potential of individual product batches.

With respect to the model-based multi-objective decision support, two aspects remain open for further development. First, the solution developed in chapters 4 and 5 does not consider a plant model mismatch that can occur during the modeling of the system or by changing due to structural modifications and aging processes. To address this a real time adjustment of the process model and the subsequent optimization process is needed. The second point for further developments was identified during the usability study in Chapter 6. Here, an increased error rate was recorded for a specific subset of the selection trials of up to 20%. Additional experiments are needed to check if the errors did occur as result of flawed experimental design or weaknesses in the design of the DSS.

The results of this thesis are a contribution towards an efficient and sustainable future of the processing industry. The resulting decision support solution can effectively monitor the process performance and enable the user to select the best operating point among the set of optimal solutions. Broadly implementing similar solutions throughout all industrial sectors can contribute to the GHG emission targets, set by the European Union.

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Appendix A

Williams-Otto parameters

Table A.1: Model parameters for the Williams-Otto semi-batch reactor.

Description	Parameter	Value	Unit
Pre–exponential coefficient reaction 1	a_1	1.6599e06	s^{-1}
Pre–exponential coefficient reaction 2	a_2	7.2117e08	s^{-1}
Pre–exponential coefficient reaction 3	a_3	2.6745e12	s^{-1}
Lumped Arrhenius parameter 1	b_1	6666.7	K
Lumped Arrhenius parameter 2	b_2	8333.3	K
Lumped Arrhenius parameter 3	b_3	11111	K
Specific heat capacity	C_P	4.184	$kJ\,(kg\ K)^{-1}$
Density	ρ	1000	kgm^{-3}
Molecular weight A, B, P	MW_A, MW_B, MW_P	100	$kg\ kmol^{-1}$
Molecular weight C,E	MW_C, MW_E	200	$kg\ kmol^{-1}$
Molecular weight G	MW_G	300	$kg\ kmol^{-1}$
Heat of reaction 1	$(-\Delta H_1)$	-263.8	$kJ\ kg^{-1}$
Heat of reaction 2	$(-\Delta H_2)$	-158.3	$kJ\ kg^{-1}$
Heat of reaction 3	$(-\Delta H_3)$	-226.3	$kJ\ kg^{-1}$
Inflow temperature	T_{in}	35	$^{\circ}C$
Reference temperature	T_{ref}	273.15	K
Final batch time	t_f	1500	s
Temperature initial condition	$T_R(t_0)$	40	$^{\circ}C$
Volume initial condition	$V(t_0)$	2	m^3
Mass A initial condition	$m_A(t_0)$	2000	kg
Mass B initial condition	$m_B(t_0)$	0	kg
Mass C initial condition	$m_B(t_0)$	0	kg
Mass E initial condition	$m_E(t_0)$	0	kg
Mass G initial condition	$m_G(t_0)$	0	kg
Mass P initial condition	$m_P(t_0)$	0	kg

Table A.2: Prices for the calculation of benefit in the Williams–Otto semi-batch reactor application case.

Description	Parameter	Value	Unit
Raw material price A	c_A	0.1509	€$/kg$
Raw material price B	c_B	0.2263	€$/kg$
Proceeds form incineration of C	c_C	0.0437	€$/kg$
Product price E	c_E	1.1315	€$/kg$
Disposal cost G	c_G	0.0754	€$/kg$
Product price P	c_P	2.2629	€$/kg$
Cooling cost	c_{QC}	0.3809e-04	€$/kW$
Heating cost	c_{QH}	0.9490e-05	€$/kW$

Appendix B

RACER evaluation WOSBR

Table B.1: RACER scores for the REIs: total material efficiency (TME), total energy efficiency (TEE), and eco-efficiency (ECO).

Category	TME	TEE	ECO
Relevant	1.75	1.75	1.75
Accepted	2	1.6	2
Credible	2	2	2
Easy	1.75	1.75	1.75
Robust	2	1.75	2

B.1 RACER evaluation TME

Name of Indicator	TME
Description (e.g. equation)	Total material efficiency: $TME = \frac{mPend + mEend}{mAges + mBges}$ Indicator is calculated at the end of teh batch
Date of Evaluation	8/19/2021
Evaluators	Marc Kalliski

Figure B.1: Summary of the RACER evaluation for the total material efficiency (TME).

Relevant				**Category average:**	**1.75**
Sub-category	Goal related	Suitable for time horizon considered (seconds / hours / campaigns)	Influenced by the actions of the operators	Transferability to other plants	
Fully achieved (2 points)	*Indicator reflects resource efficiency directly* ◉	*Indicator is meaningful for time periods of interest* ◉	*Can be influenced directly* ○	*General definition; easy to transfer* ◉	
Partially achieved (1 point)	*Indicator reflects resource efficiency indirectly* ○	*Use for short term analysis questionable (e.g. windowing effects or holdups not considered)* ○	*Possible influence but not obvious* ◉	*Tranferable with adaptations* ○	
Not achieved (0 points)	*Indicator is not related to resource efficiency* ○	*Not meaningful on short time scales* ○	*No influence* ○	*Very specific definition; not transferable* ○	
Comments	Directly reflects the ratio of invested raw material to product.	Indicator is intended for batch to batch optimization. The temporal resolution is one batch and thus sufficient.	Connection between inputs and the resulting Material efficiency is not always easy to understand, due to the relative complex reaction system	The definition of product and raw material is directly transferable to nearly all applications in the processing industry	
Points	2	2	1	2	

Figure B.2: Analysis for category "relevant" for the total material efficiency (TME).

Accepted				**Category average:**	**2**
Sub-category	Stakeholder / Higher Management	Plant Manager	Plant Operators	Academia	Public
Fully achieved (2 points)	*Widely accepted* ◉	*Widely accepted* ◉	*Widely accepted* ◉	*Widely accepted* ◉	*Widely accepted* ◉
Partially achieved (1 point)	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*New to public, known only to certain groups* ○
Not achieved (0 points)	*Strongly disputed* ○	*Strongly disputed* ○	*Strongly disputed* ○	*Strongly disputed* ○	*Not accepted / understood* ○
Comments	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance
Points	2	2	2	2	2

Figure B.3: Analysis for category "accepted" for the total material efficiency (TME).

Credible			Category average:		2
Sub-category	Consistency in direction and magnitude of movement	Unambiguous in terms of decision making	Transparency of data collection and treatment	Avoidance of double accounting regarding influences and outcomes	Clear documentation of assumptions and limitations
Fully achieved (2 points)	*Full consistency*	*Self-explanatory*	*Explicitly stated how data should be collected & which pretreatments can be applied*	*No double accounting*	*Clear and consistent definitions available*
Partially achieved (1 point)	*Consistency for main influences*	*Explanation necessary*	*Data collection and pretreatment defined to some extent but not fully*	*Minor double accounting*	*Definitions of most assumptions and limitations available*
Not achieved (0 points)	*No or very low consistency*	*Hard to understand, several meanings*	*Data collection and pretreatment left open*	*Intense double accounting*	*No documentation available*
Comments	Higher product formation and lower raw material invest improve the indicator. Magnitude scales linear with the improvement.	Self-explanatory	Well defined	No double accounting	Well defined
Points	2	2	2	2	2

Figure B.4: Analysis for category "credible" for the total material efficiency (TME).

Easy			Category average:	1.75	
Sub-category	Technical feasibility	Data availability	Automatically compiled, displayed and reported	Predictive models can be derived	
Fully achieved (2 points)	*Appropriate hard- and software is present* ◉	*Historical data available, measurements exist* ◉	*Automatic processing of measurement data and computation of the indicator seems feasible* ○	*Predictive cause-effect models are available or can be derived with moderate effort* ◉	
Partially achieved (1 point)	*Technical improvements necessary, but possible with current technology* ○	*Some data currently not recorded, but measurable* ○	*Automatic collection of required data possible but requires additional effort* ◉	*Predictive models require considerable effort* ○	
Not achieved (0 points)	*No technical solution foreseeable* ○	*Unclear how the data can be obtained* ○	*No automatic collection possible with reasonable effort* ○	*Very difficult to model* ○	
Comments	Simulation available	Simulation results available	Product amount necessary for calculation of the indicator. Might need laboratory analysis with delay	Full model exists	
Points	2	2	1	2	

Figure B.5: Analysis for category “easy” for the total material efficiency (TME).

Robust				Category average:	2
Sub-category	Theoretical background	Data quality	Reliability	System boundaries, energy and mass balances	
Fully achieved (2 points)	*No gaps and/or critical assumptions in the definition of the indicator* ◉	*Good accuracy and reproducibility of measurements* ◉	*High reliability with consistency check possible* ◉	*Closed energy and mass balances inside clear system boundaries* ◉	
Partially achieved (1 point)	*No gaps but some critical assumptions in the definition of the indicator* ○	*Medium accuracy and reproducibility, fluctuations of the indicator due to noise* ○	*High/medium reliability, no consistency check possible* ○	*Closed balances for main process and utility streams* ○	
Not achieved (0 points)	*Gaps in the definition of the indicator* ○	*Considerable fluctuations of the indicator due to noise or low accuracy of the measurement* ○	*Low reliability* ○	*Balances not closed or system boundary is unclear* ○	
Comments	Well defined assumptions and sensible interpretation possible	Exact results available	All results are documented and a consistency check can be performed (e.g. mass and energy balances)	Mass and energy balances are closed	
Points	2	2	2	2	

Figure B.6: Analysis for category "robust" for the total material efficiency (TME).

B.2 RACER evaluation TEE

Name of Indicator	TEE
Description (e.g. equation)	Total energy efficiency: mPend + mEend TEE = -------------------------------- Indicator is calculated at the end of the batch
Date of Evaluation	8/19/2021
Evaluators	Marc Kalliski

Figure B.7: Summary of the RACER evaluation for the total material efficiency (TEE).

Relevant			**Category average:**	**1.75**	
Sub-category	Goal related	Suitable for time horizon considered (seconds / hours / campaigns)	Influenced by the actions of the operators	Transferability to other plants	
Fully achieved (2 points)	*Indicator reflects resource efficiency directly* ◉	*Indicator is meaningful for time periods of interest* ◉	*Can be influenced directly* ○	*General definition; easy to transfer* ◉	
Partially achieved (1 point)	*Indicator reflects resource efficiency indirectly* ○	*Use for short term analysis questionable (e.g. windowing effects or holdups not considered)* ○	*Possible influence but not obvious* ◉	*Tranferable with adaptations* ○	
Not achieved (0 points)	*Indicator is not related to resource efficiency* ○	*Not meaningful on short time scales* ○	*No influence* ○	*Very specific definition; not transferable* ○	
Comments	Directly reflects the ratio of invested (heating/cooling) duty to product.	Indicator is intended for batch to batch optimization. The temporal resolution is one batch and thus sufficient.	Connection between inputs and the resulting Energy efficiency is not always easy to understand, due to the relative complex reaction system	The definition of product and heating and cooling duty is directly transferable to nearly all applications in the processing industry	
Points	2	2	1	2	

Figure B.8: Analysis for category “relevant” for the total material efficiency (TEE).

Accepted				**Category average:**	**1.6**
Sub-category	Stakeholder / Higher Management	Plant Manager	Plant Operators	Academia	Public
Fully achieved (2 points)	*Widely accepted* (x)	*Widely accepted* ( )	*Widely accepted* ( )	*Widely accepted* (x)	*Widely accepted* (x)
Partially achieved (1 point)	*Accepted by most experts in the domain* ( )	*Accepted by most experts in the domain* (x)	*Accepted by most experts in the domain* (x)	*Accepted by most experts in the domain* ( )	*New to public, known only to certain groups* ( )
Not achieved (0 points)	*Strongly disputed* ( )	*Strongly disputed* ( )	*Strongly disputed* ( )	*Strongly disputed* ( )	*Not accepted / understood* ( )
Comments	Heating and cooling duty is perceived as investment into the process	Heating and cooling has different prices. equal consideration is counter intuitive at first. Weighting possible	Heating and cooling has different prices. equal consideration is counter intuitive at first. Weighting possible	Simplification of equal weights for heating and cooling duties is reasonable	Simplification of equal weights for heating and cooling duties is reasonable
Points	2	1	1	2	2

Figure B.9: Analysis for category "accepted" for the total material efficiency (TEE).

Credible			Category average:		2
Sub-category	Consistency in direction and magnitude of movement	Unambiguous in terms of decision making	Transparency of data collection and treatment	Avoidance of double accounting regarding influences and outcomes	Clear documentation of assumptions and limitations
Fully achieved (2 points)	*Full consistency* ◉	*Self-explanatory* ◉	*Explicitly stated how data should be collected & which pretreatments can be applied* ◉	*No double accounting* ◉	*Clear and consistent definitions available* ◉
Partially achieved (1 point)	*Consistency for main influences* ○	*Explanation necessary* ○	*Data collection and pretreatment defined to some extent but not fully* ○	*Minor double accounting* ○	*Definitions of most assumptions and limitations available* ○
Not achieved (0 points)	*No or very low consistency* ○	*Hard to understand, several meanings* ○	*Data collection and pretreatment left open* ○	*Intense double accounting* ○	*No documentation available* ○
Comments	Higher product formation and lower energy invest improves the indicator. Magnitude scales linear with the improvement.	Self-explanatory	Well defined	No double accounting	Well defined
Points	2	2	2	2	2

Figure B.10: Analysis for category “credible” for the total material efficiency (TEE).

Easy			Category average:	1.75	
Sub-category	Technical feasibility	Data availability	Automatically compiled, displayed and reported	Predictive models can be derived	
Fully achieved (2 points)	*Appropriate hard- and software is present* ●	*Historical data available, measurements exist* ●	*Automatic processing of measurement data and computation of the indicator seems feasible* ○	*Predictive cause-effect models are available or can be derived with moderate effort* ●	
Partially achieved (1 point)	*Technical improvements necessary, but possible with current technology* ○	*Some data currently not recorded, but measurable* ○	*Automatic collection of required data possible but requires additional effort* ●	*Predictive models require considerable effort* ○	
Not achieved (0 points)	*No technical solution foreseeable* ○	*Unclear how the data can be obtained* ○	*No automatic collection possible with reasonable effort* ○	*Very difficult to model* ○	
Comments	Simulation available	Simulation results available	Product amount necessary for calculation of the indicator. Might need laboratory analysis with delay	Full model exists	
Points	2	2	1	2	

Figure B.11: Analysis for category “easy” for the total material efficiency (TEE).

Robust				Category average:	1.75
Sub-category	Theoretical background	Data quality	Reliability	System boundaries, energy and mass balances	
Fully achieved (2 points)	*No gaps and/or critical assumptions in the definition of the indicator* ○	*Good accuracy and reproducibility of measurements* ◉	*High reliability with consistency check possible* ◉	*Closed energy and mass balances inside clear system boundaries* ◉	
Partially achieved (1 point)	*No gaps but some critical assumptions in the definition of the indicator* ◉	*Medium accuracy and reproducibility, fluctuations of the indicator due to noise* ○	*High/medium reliability, no consistency check possible* ○	*Closed balances for main process and utility streams* ○	
Not achieved (0 points)	*Gaps in the definition of the indicator* ○	*Considerable fluctuations of the indicator due to noise or low accuracy of the measurement* ○	*Low reliability* ○	*Balances not closed or system boundary is unclear* ○	
Comments	Not differentiating between heating and cooling duty can be seen critical	Exact results available	All results are documented and a consistency check can be performed (e.g. mass and energy balances)	Mass and energy balances are closed	
Points	1	2	2	2	

Figure B.12: Analysis for category “robust” for the total material efficiency (TEE).

B.3 RACER evaluation ECO

Name of Indicator	ECO
Description (e.g. equation)	Total material efficiency: $ECO = \frac{mPend + mEend}{mGend}$ Calculated at the end of the batch
Date of Evaluation	8/19/2021
Evaluators	Marc Kalliski

Figure B.13: Summary of the RACER evaluation for the total material efficiency (ECO).

Relevant			**Category average:**	1.75	
Sub-category	Goal related	Suitable for time horizon considered (seconds / hours / campaigns)	Influenced by the actions of the operators	Transferability to other plants	
Fully achieved (2 points)	*Indicator reflects resource efficiency directly* ●	*Indicator is meaningful for time periods of interest* ●	*Can be influenced directly* ○	*General definition; easy to transfer* ●	
Partially achieved (1 point)	*Indicator reflects resource efficiency indirectly* ○	*Use for short term analysis questionable (e.g. windowing effects or holdups not considered)* ○	*Possible influence but not obvious* ●	*Tranferable with adaptations* ○	
Not achieved (0 points)	*Indicator is not related to resource efficiency* ○	*Not meaningful on short time scales* ○	*No influence* ○	*Very specific definition; not transferable* ○	
Comments	Directly reflects the ratio of toxic side product to product.	Indicator is intended for batch to batch optimization. The temporal resolution is one batch and thus sufficient.	Connection between inputs and the resulting Material efficiency is not always easy to understand, due to the relative complex reaction system	The definition of product and side product with environmental impact are directly transferable to nearly all applications in the processing industry	
Points	2	2	1	2	

Figure B.14: Analysis for category “relevant” for the total material efficiency (ECO).

Accepted			**Category average:**		2
Sub-category	Stakeholder / Higher Management	Plant Manager	Plant Operators	Academia	Public
Fully achieved (2 points)	*Widely accepted* ●	*Widely accepted* ●	*Widely accepted* ●	*Widely accepted* ●	*Widely accepted* ●
Partially achieved (1 point)	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*Accepted by most experts in the domain* ○	*New to public, known only to certain groups* ○
Not achieved (0 points)	*Strongly disputed* ○	*Strongly disputed* ○	*Strongly disputed* ○	*Strongly disputed* ○	*Not accepted / understood* ○
Comments	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance	Simplicity of the indicator is cause for the assumption of full acceptance
Points	2	2	2	2	2

Figure B.15: Analysis for category “accepted” for the total material efficiency (ECO).

Credible			Category average:		2
Sub-category	Consistency in direction and magnitude of movement	Unambiguous in terms of decision making	Transparency of data collection and treatment	Avoidance of double accounting regarding influences and outcomes	Clear documentation of assumptions and limitations
Fully achieved (2 points)	*Full consistency* ◉	*Self-explanatory* ◉	*Explicitly stated how data should be collected & which pretreatments can be applied* ◉	*No double accounting* ◉	*Clear and consistent definitions available* ◉
Partially achieved (1 point)	*Consistency for main influences* ○	*Explanation necessary* ○	*Data collection and pretreatment defined to some extent but not fully* ○	*Minor double accounting* ○	*Definitions of most assumptions and limitations available* ○
Not achieved (0 points)	*No or very low consistency* ○	*Hard to understand, several meanings* ○	*Data collection and pretreatment left open* ○	*Intense double accounting* ○	*No documentation available* ○
Comments	Higher product formation and lower side product formation improve the indicator. Magnitude scales linear with the improvement.	Self-explanatory	Final composition necessary for calculation of the indicator. Might need laboratory analysis with delay	No double accounting	Well defined
Points	2	2	2	2	2

Figure B.16: Analysis for category “credible” for the total material efficiency (ECO).

Easy			Category average:	1.75	
Sub-category	Technical feasibility	Data availability	Automatically compiled, displayed and reported	Predictive models can be derived	
Fully achieved (2 points)	*Appropriate hard- and software is present* ◉	*Historical data available, measurements exist* ◉	*Automatic processing of measurement data and computation of the indicator seems feasible* ○	*Predictive cause-effect models are available or can be derived with moderate effort* ◉	
Partially achieved (1 point)	*Technical improvements necessary, but possible with current technology* ○	*Some data currently not recorded, but measurable* ○	*Automatic collection of required data possible but requires additional effort* ◉	*Predictive models require considerable effort* ○	
Not achieved (0 points)	*No technical solution foreseeable* ○	*Unclear how the data can be obtained* ○	*No automatic collection possible with reasonable effort* ○	*Very difficult to model* ○	
Comments	Simulation available	Simulation results available	Product amount necessary for calculation of the indicator. Might need laboratory analysis with delay	Full model exists	
Points	2	2	1	2	

Figure B.17: Analysis for category “easy” for the total material efficiency (ECO).

Robust				**Category average:**	**2**
Sub-category	Theoretical background	Data quality	Reliability	System boun-daries, energy and mass balances	
Fully achieved (2 points)	*No gaps and/or critical assumptions in the definition of the indicator*	*Good accuracy and reproducibility of measurements*	*High reliability with consistency check possible*	*Closed energy and mass balances inside clear system boundaries*	
Partially achieved (1 point)	*No gaps but some critical assumptions in the definition of the indicator*	*Medium accuracy and reproducibility, fluctuations of the indicator due to noise*	*High/medium reliability, no consistency check possible*	*Closed balances for main process and utility streams*	
Not achieved (0 points)	*Gaps in the definition of the indicator*	*Considerable fluctuations of the indicator due to noise or low accuracy of the measurement*	*Low reliability*	*Balances not closed or system boundary is unclear*	
Comments	Well defined assumptions and sensible interpretation possible	Exact results available	All results are documented and a consistency check can be performed (e.g. mass and energy balances)	Mass and energy balances are closed	
Points	2	2	2	2	

Figure B.18: Analysis for category “robust” for the total material efficiency (ECO).

Appendix C

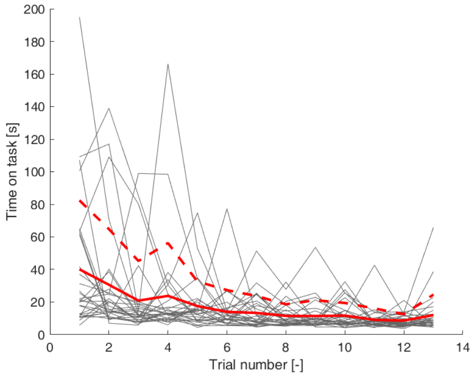
Usability study

Table C.1: German SUS-survey questions as translated based on the publication by Brooke (1996).

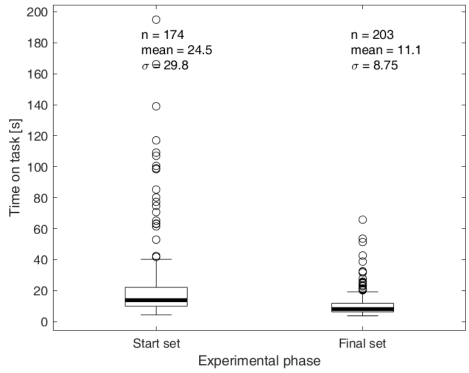
Number	Question
1.	Ich kann mir gut vorstellen, das Decision Support Tool regelmäßig zu nutzen.
2.	Ich empfinde das Decision Support Tool als unnötig komplex.
3.	Ich empfinde das Decision Support Tool als einfach zu nutzen.
4.	Ich denke, dass ich technischen Support brauchen würde, um das Decision Support Tool zu nutzen.
5.	Ich finde, dass die verschiedenen Funktionen gut integriert sind.
6.	Ich finde, dass es im Decision Support Tool zu viele Inkonsistenzen gibt.
7.	Ich kann mir vorstellen, dass die meisten Leute das System schnell zu beherrschen lernen.
8.	Ich empfinde die Bedienung als sehr umsändlich.
9.	Ich habe mich bei der Nutzung sicher gefühlt.
10.	Ich musste eine Menge lernen, bevor ich mit dem System arbeiten konnte.

Table C.2: Participant demographics for the expert interviews of dashboard alternative one.

Participant	Age	Gender	Level of education	Expertise
1	30	male	MSc	Chemical Engineering
2	25	female	MSc	Chemical Engineering
3	32	male	Dipl.Ing	Mechanical Engineering
4	30	male	MSc	Automation and Robotics
5	24	male	MSc	Chemical Engineering

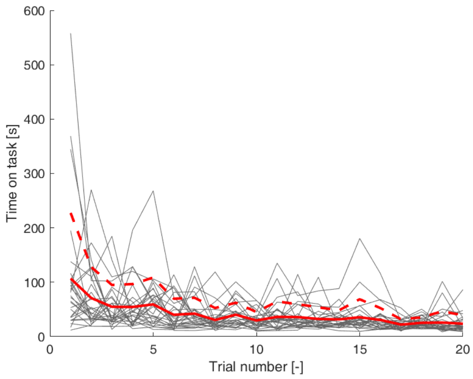


(a) Time on task over individual trial number for type 1 – category one trials.

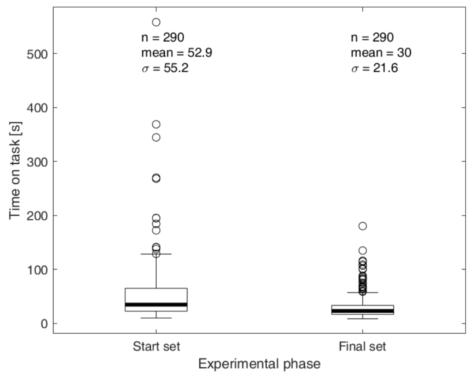


(b) Comparison of the starting and final set regarding time on task for type 1 – category one trials.

Figure C.1: Type 1 learning assessment for category one trials.

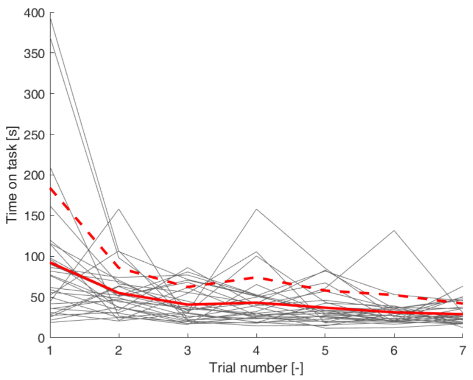


(a) Time on task over individual trial number for type 1 – category two trials.

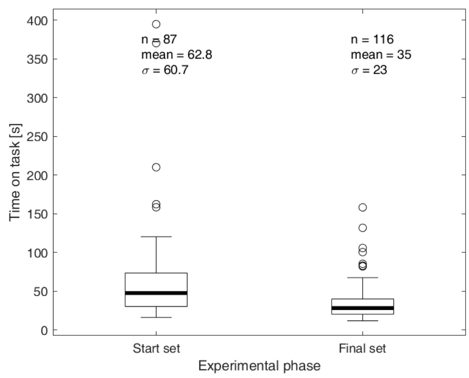


(b) Type 1 learning assessment for category two trials.

Figure C.2: Type 1 learning assessment for category two trials.

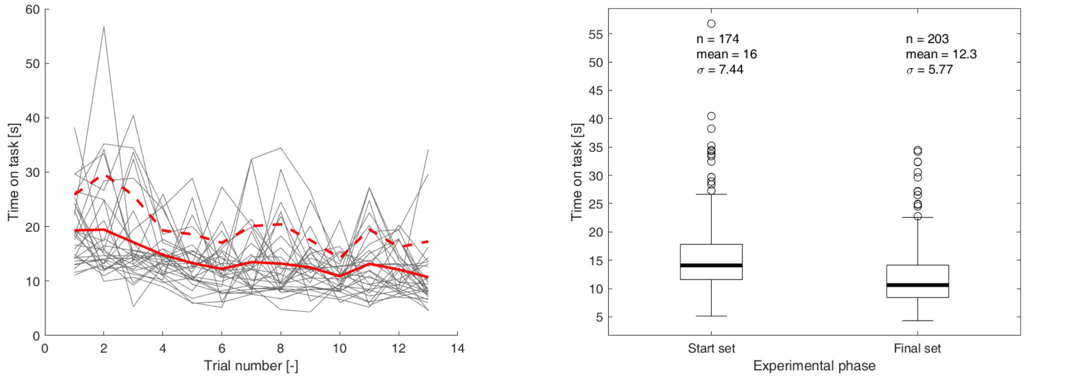


(a) Time on task over individual trial number for type 1 – category three trials.



(b) Type 1 learning assessment for category three trials.

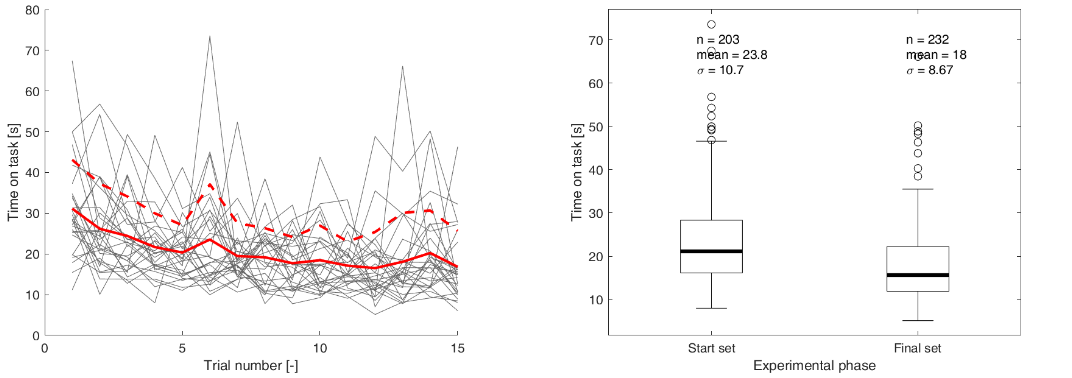
Figure C.3: Type 1 learning assessment for category three trials.



(a) Time on task over individual trial number for type 2 – category one trials.

(b) Type 2 learning assessment for category one trials.

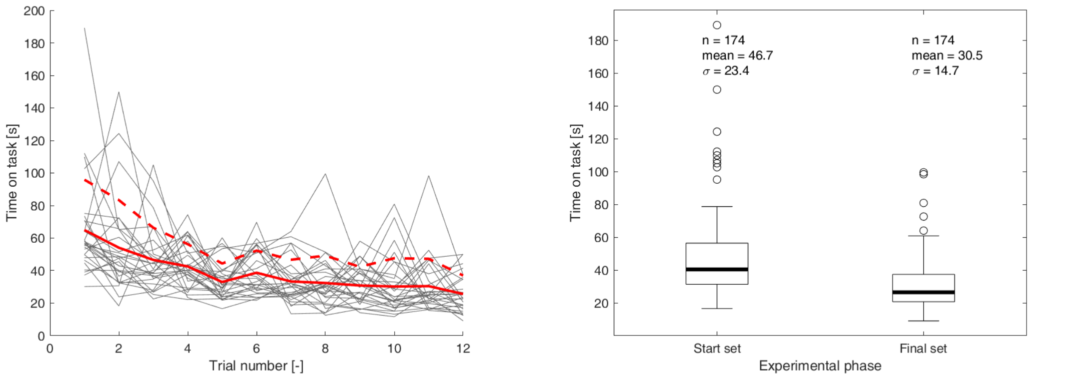
Figure C.4: Type 2 learning assessment for category one trials.



(a) Time on task over individual trial number for type 2 – category two trials.

(b) Type 2 learning assessment for category two trials.

Figure C.5: Type 2 learning assessment for category two trials.



(a) Time on task over individual trial number for type 2 – category three trials.

(b) Type 2 learning assessment for category three trials.

Figure C.6: Type 2 learning assessment for category three trials.