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Value Stream Mapping and Discrete Event Simulation for Optimization of Chemical Production Processes

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Abstract

Over the past 15 years, Value Stream Mapping (VSM) has emerged as the predominant Lean implementation method within the manufacturing industry. The secret of its success is rooted in the holistic approach and, at the same, the straightforwardness which allows for engagement of all stakeholders along the value stream. These attributes of the “paper and pencil” method, however, result in limitations when applying VSM in complex production environments, as particularly found in the chemical industry. Upon closer inspection, VSM lacks the ability to adequately capture complex process routing and to account for process variability. In those environments, it further fails to prove feasibility and to reliably quantify the actual benefit of proposed future states prior to implementation of the improvement measures. In this thesis, these shortcomings are tackled through enhancement of the method with the aid of Discrete Event Simulation (DES). The outcome is a VSM approach, which is capable of predicting feasibility and benefit of proposed future states in complex chemical production environments. In addition, the applicability of DES for modelling chemical production processes is explored beyond its deployment in VSM projects. Integration of DES with Discrete Rate Simulation and continuous simulation is elaborated, in order to account for peculiarities of chemical production. The benefit of the simulation technique, which has only been applied scarcely in the chemical industry to date, is demonstrated for holistic operating cost optimization as well as debottlenecking of transient mixed batch-continuous chemical production processes.

Kurzzusammenfassung

In den vergangenen 15 Jahren hat sich die Wertstromanalyse als bevorzugte Lean-Implementierungsmethode der Industrie etabliert. Der Hauptgrund für die weite Verbreitung der Methode liegt in ihrer Ganzheitlichkeit und Geradlinigkeit, die es ermöglicht, alle in eine Prozesskette involvierten Personen in das Wertstromanalysen-Projekt zur Lean-Implementierung einzubinden. Diese Eigenheit der Methode, für welche keine besonderen technischen Hilfsmittel benötigt werden, führt allerdings zu Limitierungen bei deren Anwendung auf komplexe Produktionssysteme, wie sie beispielsweise häufig in der chemischen Industrie zu finden sind. Bei genauerer Betrachtung stellt man fest, dass durch die Wertstromanalyse komplexe Prozessführungen sowie Variabilität nicht abgebildet werden können. Darüber hinaus ist es während eines Wertstromanalysen-Projekts oft nicht möglich, die technische Umsetzbarkeit und den monetären Nutzen des auf dem Papier optimierten Prozesses vor der Implementierung verlässlich vorherzusagen. In der vorliegenden Arbeit wird die Methode mit Hilfe von Discrete Event Simulation (DES) so modifiziert, dass auch komplexe Produktionssysteme analysiert und die Umsetzbarkeit sowie der Nutzen eines Optimierungsvorschlags vorab bewertet werden können. Zusätzlich wird die Anwendbarkeit von DES über den Einsatz in Wertstromanalysen-Projekten hinaus zur Modellierung und Optimierung chemischer Prozesse untersucht. Hierbei wird DES mit Discrete Rate Simulation und kontinuierlichen Simulationstechniken kombiniert, um die Besonderheiten von chemischen Produktionsprozessen adäquat abbilden zu können. Der Nutzen des Simulationsansatzes, welcher bisher kaum in der chemischen Industrie Anwendung gefunden hat, wird anhand eines Projekts zur ganzheitlichen Kostenoptimierung sowie eines Projekts zur Durchsatzoptimierung, jeweils für einen instationären chemischen Prozesses bestehend aus verschiedenen kontinuierlichen und chargenweise betriebenen Verfahrensschritten, gezeigt.

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Abbreviations

DES	Discrete Event Simulation
DOE	Design Of Experiments
DRS	Discrete Rate Simulation
ES	Evolutionary Strategies
FIFO	First In First Out
I	Inventory
IID	independent and identically distributed
JIT	Just In Time
pc	Piece
PGM	Platinum Group Metals
SCM	Supply Chain Management
SCR	Selective Catalytic Reduction
SME	Subject Matter Expert (process expert, who provides input data for a Discrete Event Simulation model)
SMED	Single-Minute Exchange of Die
TPM	Total Productive Maintenance
TPS	Toyota Production System
VSM	Value Stream Mapping

Symbols

Formula symbols

ATC	Average total costs	€ kg^{-1} or € pc^{-1}
BS	Batch size	kg or pcs
BT	Batch time	s
COT	Changeover time	s
CT	Cycle time	s kg^{-1} or s pc^{-1}
DDLT	Demand during lead time	kg or pcs
EPEx	Every part every interval	h
f	Mass correction factor	-
FR	Flow ratio	-
FWD	Factory working days	d a^{-1}
LT	Labour time	h d^{-1}
m	Mass	kg
MC	Marginal costs	€ kg^{-1} or € pc^{-1}
OEE	Overall equipment effectiveness	-
PLT	Process lead time	d
PT	Process time	s
q	Quantity	diverse, e.g. kg, pc, or kWh
RMLT	Raw material lead time	h
t	Time	s
TT	Takt time	h kg^{-1} or h pc^{-1}
V	Volume	m^3
WIP	Work in process	kg or pcs

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cc	Cost component
p	Product

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1 Introduction

1.1 The evolution of production systems – from craft to Lean production

In an ever globalising business environment, economic competitiveness is key for the success of any manufacturing company. Enterprises strive for customer oriented, cost efficient production systems to prevail within their market segment.

At the beginning of the 20th century, many manufacturers achieved a competitive edge through mass production systems. Headed by the Ford Motor Company, assembly line processes were introduced, which allowed for high volume production, driving down costs through economies of scale (Maxcy and Silberston 1959). Mass producers installed special purpose machines which were located according to production sequence, opening up the possibility to employ unskilled workers (Hounshell 1984). Assembly lines drastically reduced motion within the plant and established stable production rates. These developments opened up a significant productivity gap and helped mass producers outperform pre-industrialized craft producers (Krafcik 1988).

However, over the course of the 20th century, several weaknesses of the first mass production systems became evident. Specially designed single purpose machinery inevitably led to inflexible production processes and, consequently, to restricted product portfolios. Changeovers were costly and time consuming procedures. For instance, Ford's transition of their production lines to produce Model A instead of Model T took six months (Hounshell 1984). What's more, as production processes were broken down into a multitude of worker tasks along the assembly line of perhaps only 30 seconds (Krafcik 1988), high amounts of unfinished material were present on the shop floor. This effect was even amplified, as safety buffers were installed to prevent individual machine breakdowns from obstructing the whole production line.

Taiichi Ohno from Toyota recognised two major flaws in western manufacturing companies. First, production in large batches due to inflexible processes resulted in inevitable creation of high inventories, which took up costly capital and warehouse space. This also led to permanently high defect rates, because of delayed identification of process deterioration. Second, also caused by inflexible high inventory processes, western producers were not able to meet customer preferences for product diversity (Ohno 1988). Ohno's findings majorly contributed to the development of the Toyota Production System (TPS) that managed to combine the strengths of both mass and craft producers (Womack, Jones and Roos, D., 1990). TPS was built on the two pillars Just In Time (JIT) – the arrival of material at the right time only to the right amount, and Jidoka – ‘intelligent automation’ of process equipment (Ohno 1988). In contrast to mass producers, TPS did not rely on cost reduction through high as possible production rates, but production cycle times equal to the so called takt time (TT) predefined by the customer demand. Instead of highly specialized machines, TPS promoted cross training of workers, who were able to perform maintenance and quality control tasks at their less sophisticated but more flexible production machines (Womack, Jones and Roos, D., 1990). Furthermore, Toyota established a culture of continuous improvement throughout their workforce in order to strive for elimination of all non-value added activities. Over the course of the 20th century, Japanese companies outperformed western producers with what is nowadays termed Lean production. Through the developments of TPS, they were able keep inventory and defect rates low and at the same time produce a high variety of products.

The advantage of Toyota and other Japanese manufacturing companies was soon recognized by western industries and research facilities. Extensive research initiatives were brought to life, such as the International Motor Vehicle Program (IMVP) founded at the Massachusetts Institute of Technology in 1979, in order to understand the advantages of Japanese production techniques and to exploit their benefits (Holweg 2007). The key finding of the IVMP was conveyed by Krafcik (1988), who concluded that what was formerly termed ‘fragile production’ (no big buffers of intermediates in between process steps) worked out as an advantage for TPS. Therefore, the negative term ‘fragile’ was substituted by the more positive sounding term ‘lean’. The final breakthrough of the Lean production paradigm came with the book The Machine that Changed the World (Womack, Jones, and Roos 1990), in which the gap between former western mass production and Lean production is highlighted.

Starting in the 1980s, the Japanese production techniques have been popularized throughout the manufacturing sector. Based on TPS, several other concepts were introduced alongside Lean production, such as zero inventory production (Hall 1983), world class manufacturing (Schonberger 1986) or continuous flow manufacturing (Beal 1988). Today, Lean production is a well-established subject of academic literature. A concise review of the development of Lean production from its roots in TPS to a globally deployed process improvement concept is presented by Holweg (2007). A literature-based taxonomy of the wide field of Lean is provided by Taylor, Taylor and

McSweeney (2013) Upon further interest on the evolution of Lean thinking alongside its increasing popularity, see Hines, Holweg and Rich (2004).

However, despite its high diffusion, counter-arguments against Lean production have arisen. Limitations of Lean have been reported in sectors that are different from its original field of application in the manufacturing sector (Marodin and Saurin 2013). Krafcik (1988) concluded in analogy to the world of finance, that Lean production has high risks (shutdown of one machine leads to breakdown of the whole line), but on the other hand yields high return (low production costs due to low inventory when the line is running). Inconsiderately following the Lean approach by continuous batch size reduction or strict JIT policies can become disadvantageous if changeover efforts are irrepressible or supply chains are unstable. The latter is very likely if, for instance, suppliers are geographically dispersed (Cusumano 1994). The risk of Lean systems is particularly high in production environments with low demand predictability and a high variety of products with low volumes (Christopher 2000). Others point out the continuing importance of economies of scale for competitiveness, for instance in the automotive industry (Husan 1997). Hayes and Pisano (1994) emphasize that there is not one best way for designing production systems and that thorough selection among production techniques depending on an enterprise's surrounding conditions is key for success. This thesis is supported by Bertolini et al. (2013), who proved that the pure material pull approach of Lean may not be optimal in high variety low volume manufacturing facilities.

1.2 Goals, principles and tools of Lean production

Taiichi Ohno defined seven kinds of waste, which TPS strives to eliminate (John et al. 2008). Table 1 summarizes these wastes, their primary effect as well as their interconnection. Analysis shows, that improving workforce utilization is a key element of successful Lean implementation. The central waste, however, is 'inventory' (Ohno 1988). The wastes 'transport', 'motion' and 'waiting' facilitate build-up of inventory, which hides inefficiencies in the process. 'Inventory' itself facilitates 'overproduction', because high amounts of semi-finished and final products on stock can end up useless when customer demand changes. Furthermore, it raises the risk of high defect rates, as process deterioration may be detected in delay, or not at all.

Table 1: Seven types of waste and their effects.

Waste	Primary effect	Dependent wastes
Transport	Inefficient workforce utilization	Inventory
Inventory	Tied capital/storage costs	Overproduction, defects
Motion	Inefficient workforce utilisation	Inventory
Waiting	Inefficient workforce/equipment utilisation	Inventory
Overproduction	Excess expenses	
Overprocessing	Excess expenses	
Defects	Excess expenses	

When analysing the principles and tools, with which Lean producers seek to reduce waste, one has to distinguish between cultural and technical Lean methods. The keyword for cultural Lean implementation is the Japanese Kaizen, which means ‘change to the better’. It represents a culture of continuous improvement, in which all employees throughout the hierarchical system of the company are motivated to question processes and find ways to optimize them. It also gives high responsibility to the production work force. The related Total Productive Maintenance (TPM) for instance engages production shift works in the maintenance of equipment to increase its availability. Furthermore, emphasis is put on the importance of involving all employees in solving quality issues in order to decrease defect rates. In contrast, traditional western production systems rely on separate quality departments, which determine defects in delay and are less likely to determine root causes due to their distance from the process. The applicability of Kaizen in western companies has been questioned largely because of cultural differences to the Japanese. However research suggests that it is less an issue of national culture than organisational culture and that with some effort successful implementation is possible (Recht and Wilderom 1998).

On the technical side, the two pillars of TPS, JIT and Jidoka, are filled with several tools, which all contribute to reduction of waste as defined by Taiichi Ohno. A selection is listed and briefly introduced below:

– *Takt time pacing*:
  A central target of Lean production is synchronization of each work step throughout the process with the takt time (TT), as defined in Eq. 1. The term is derived from the German word “Takt”, which was used to set the pace of production for the German aircraft industry in the 1930s (Ohno 1988). Through

orientation towards TT, predominantly, overproduction is tackled. It is made sure that no process step is running ahead and that the customer demand is exactly met.

$$TT = \frac{available\ production\ time}{output\ number\ demanded\ by\ customer} \qquad \text{Eq. 1}$$

- *Cellular manufacturing*:
  In order to facilitate continuous flow as well as worker involvement in the continuous improvement process, production processes are rearranged and work steps are grouped in cells according to product families instead of machine type. For an introduction to scientific approaches to cellular manufacturing, see the review by Singh (1993).
- *Pull systems*:
  JIT production is largely supported by the introduction of pull systems. Instead of applying central planning for all process resources, a self-regulated system is introduced. While ideally only one process step is centrally scheduled according to TT, material of all upstream steps is requested, or 'pulled' when inventory falls below a critical level. The method has been refined through the introduction of co-called Kanban supermarkets (Monden 1981).
- *Levelled and mixed model production*:
  In order to achieve flexibility, Lean production demands that only small increments of production volumes are released for processing. By placing small production orders in so-called Heijunka boxes, an even production flow of all product types is generated (Coleman, Vaghefi and Reza 1994).
- *Poka Yoke*:
  For error prevention, TPS introduced Poka Yoke, which essentially means making processes fool-proof. Processes are analysed for any weaknesses and physical properties are added to either product or equipment to rule out errors (Shingo 1986).
- *Single minute exchange of die (SMED)*:
  As many other Lean tools entail the obvious disadvantage of increasing the number of changeover efforts, TPS advocates reduction of changeovers through SMED. When applying the method, the changeover process is analysed in detail

and as much effort as possible is shifted from the changeover itself to the time when production is still running (Shingo 1983).

With the proliferation of Lean production, many of the principles and tools were integrated into western production systems. Alongside the popularisation of Lean production, further methods have been developed. Perhaps the most popular method is Value Stream Mapping (VSM), which was introduced by the Lean Enterprise Institute. VSM is a holistic approach for Lean implementation, which entails several of the tools outlined above (Rother and Shook 1999). It is presented in detail in Section 3.

1.3 Lean production in the chemical industry

The development of production systems from craft over mass to Lean production originated in the automotive industry and spread throughout the manufacturing sector. However, one segment that has not quite followed the developments is the chemical industry. Numerous articles and reports can be found on the deployment of Lean production across discrete part manufacturing segments, but the coverage of its application in the chemical industry has been scarce (King 2009). There are several reasons for this gap.

Options for rearranging chemical production processes are certainly more limited than for rearranging assembly line processes: Process steps are connected through pipes and vessels with fixed capacity (Anvar and Irannejad 2010). Also, process equipment may be suited for single purpose use only. Furthermore, changeover efforts are typically higher in chemical processes than in assembly lines (Russel 2012, Bretzke 2012). Reducing batch sizes may not only cause time loss, but also increase energy and material consumption due to process start-up or costly waste water generation. Another distinction between chemical and assembly line processes is the general flow pattern. While in assembly plants flow mostly converges, as numerous components are used to produce a small range of final products, the opposite is the case in chemical plants (Umble and Srikanth 1990). Chemical production distinguishes itself by a small range of raw materials and a wide variety of final products. This makes establishing JIT pull systems at the customer end of the processes far more challenging. Moreover, chemical production rather tends to be capital intensive than labour intensive (King 2009). Achieving optimum workforce utilisation, as propagated by Lean supporters is actually not fruitful in many chemical plants. Commonly, throughput is limited by equipment and not by labour in the chemical industry. Consequently, optimization projects in chemical plants often target capacity increase and debottlenecking of process equipment. Figure 1 shows an exemplary distribution of direct costs of a catalyst produced by Clariant. Besides raw material, the dominating cost contributor is plant depreciation (22.8 %). Labour only accounts for 12.8 % of the costs. Figure 2 on the other hand displays the distribution of direct costs, excluding R&D and administration overhead in the automotive industry (Becker 2007). While depreciation only plays a minor role (7.1 %), the share of labour costs (25.0 %) is by a considerable margin higher than in the chemical process. Labour costs are even amplified, if the supply chain is taken into account. Since vertical integration is low in the automotive industry, the raw material share actually contains a substantial amount of labour costs. Throughout the supply chain, it is estimated that labour makes up 65 % of total production costs in the automotive industry (Baum and Delfmann 2010). Another distinction between chemical and automotive production, which can be identified when comparing Figure 1 and Figure 2, is the cost share of energy and waste water. In the chemical process, energy and waste water costs are roughly of the same magnitude as labour costs. In automotive production however, energy and waste water costs are not even separately mentioned.

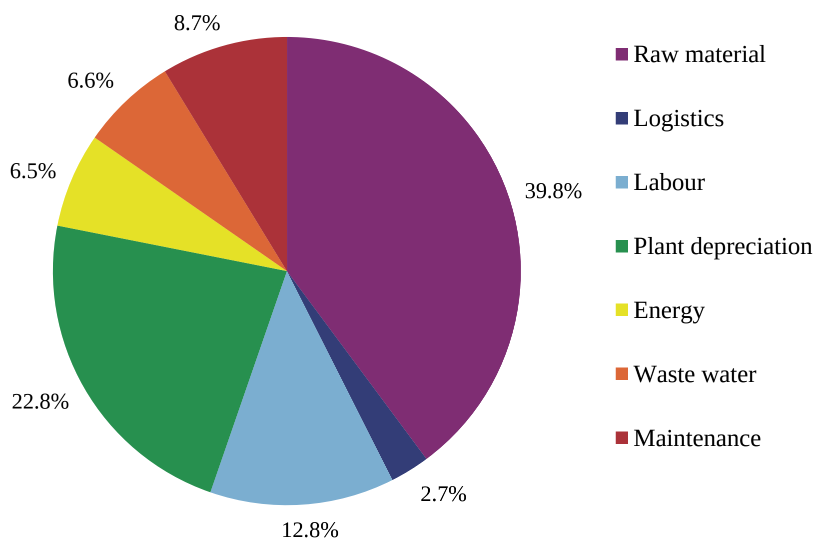


Figure 1: Cost distribution of a precipitation catalyst produced by Clariant.

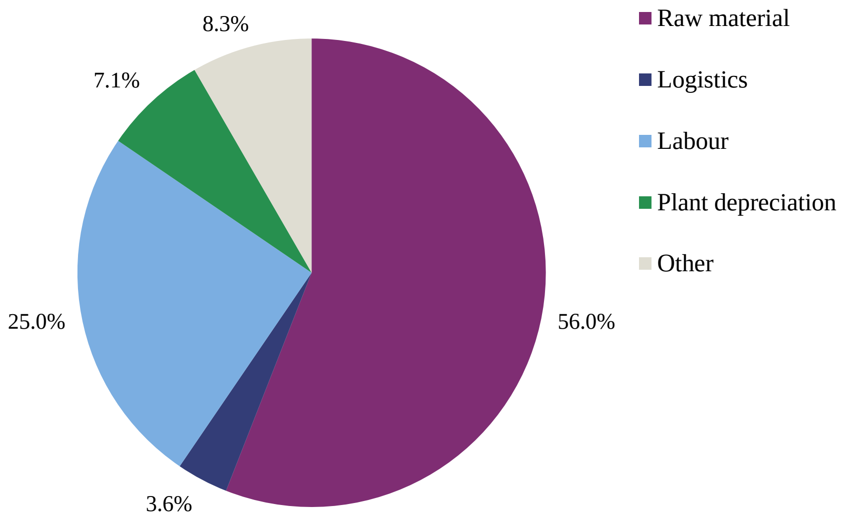


Figure 2: Cost distribution in the automotive industry production (Becker 2007).

In summary, the following obstacles restrain the chemical industry from fully adopting the Lean philosophy:

- There are less rearrangement options due to less flexible processes
- Higher changeovers efforts impede batch size reduction
- Diverging flow patterns complicate implementation at the customer end
- Trade-offs between Lean goals and other optimization goals, such as low energy and material consumption are mostly not negligible
- Lean goals may be secondary to other optimization goals

Nevertheless, to some extent, gainful Lean implementation has been reported in the chemical and process industry. Melton (2005) states that, although not yet widely spread, Lean transformation is capable of releasing working capital, increasing supply chain speed and reducing manufacturing costs in the process industry. Bretzke (2012) on the other hand advances a more sceptical view and claims Lean is not well-suited for improvement inside a chemical plant, but only between companies through Lean supply chain management. Lyons et al. (2013) conclude from a large scale case study, that general continuous waste reduction as propagated by Lean is well established within the process industry, however application of other Lean principles is less common. A similar view is presented by Russel (2012), who stresses the gainful impact of continuous improvement. Pool, Wijngaard and van der Zee (2011) successfully implemented cyclic scheduling for obtaining a pull production process in a mixed continuous-discrete food processing plant. Detailed analysis of Lean optimization techniques as well as their suitability for various types of process environments is provided by Abdulmalek, Rajgopal and LaScola Needy (2006). King (2009) even presents a detailed textbook on how to approach Lean implementation in the process industry. Furthermore, to some extent, the lean philosophy is nowadays integrated in the data driven optimization approach Six Sigma, which is being largely implemented in the chemical industry. For an introduction to the Lean Sigma or Lean Six Sigma approach, see John et al. (2008).

1.4 Scope and structure of this thesis

In this thesis, the applicability of Lean production in the chemical industry through VSM is analysed. In Section 2, optimization goals in the chemical industry are presented in detail and compared to the primary goals of Lean production. In an analytical approach, the optimization goals are translated into cost components which serve as the basis for quantifying the benefit of Lean implementation. Consecutively, options are discussed about how to couple process parameters to the cost components. Section 3 provides an introduction to the Lean implementation method VSM, as well as a literature review about its application. In Section 4, Discrete Event Simulation (DES) is introduced, a tool which may be utilized to overcome weaknesses of VSM. For this purpose, a DES enhanced VSM method is developed. Furthermore, options to couple DES with Discrete Rate Simulation (DRS) as well as continuous simulation are evaluated in order to adapt the method to chemical processes. In Section 5 several case studies are presented, with which the applicability of VSM and DES in practice is analysed. Except for case study 3, which is a model process, all case studies are based on real production processes in the Clariant business unit Catalysts. Case study 1 covers the application of VSM in a catalytic converter process. In case study 2, the applicability of DES enhanced VSM is validated in a more complex catalytic converter production process. In case study 3, the adaption of DES to chemical processes is presented in detail in a model precipitation process. Finally, in case study 4, the adapted DES approach is applied beyond Lean production. The method is utilised for the classical chemical engineering problem of debottlenecking in a complex multi-stage waste water process.

2 Optimization in the chemical industry

2.1 Economical aspects of chemical production processes

The ultimate aim of any private enterprise is to make profit. For survival in free market environments, it is mandatory to prevail against competitors. Only profitable companies are able to attract investors to provide capital and, hereby, to continue their business. In the chemical industry, value is created by converting raw materials into chemical products through miscellaneous operations.

The revenue of chemicals sold has to exceed numerous cost components in order to achieve positive cash flow in the long term and to continue the company’s operations. A simplified overview of the cash flow cycle in industrial operations is presented in Figure 3. Capital is required for investment in plants as well as material inventory. Based on these investments, chemicals are produced at the expense of various operating costs. The gross profit, calculated from sales revenue less operating costs and capital investment depreciation, is subject to income tax, leaving the net profit. The net profit plus depreciation yields net cash flow from operations into the company’s capital, which is required for repayment and interest of invested capital. Finally, surpluses are utilised for stockholder dividends to raise attractiveness for investors and gain further capital for maintaining and expanding operations.

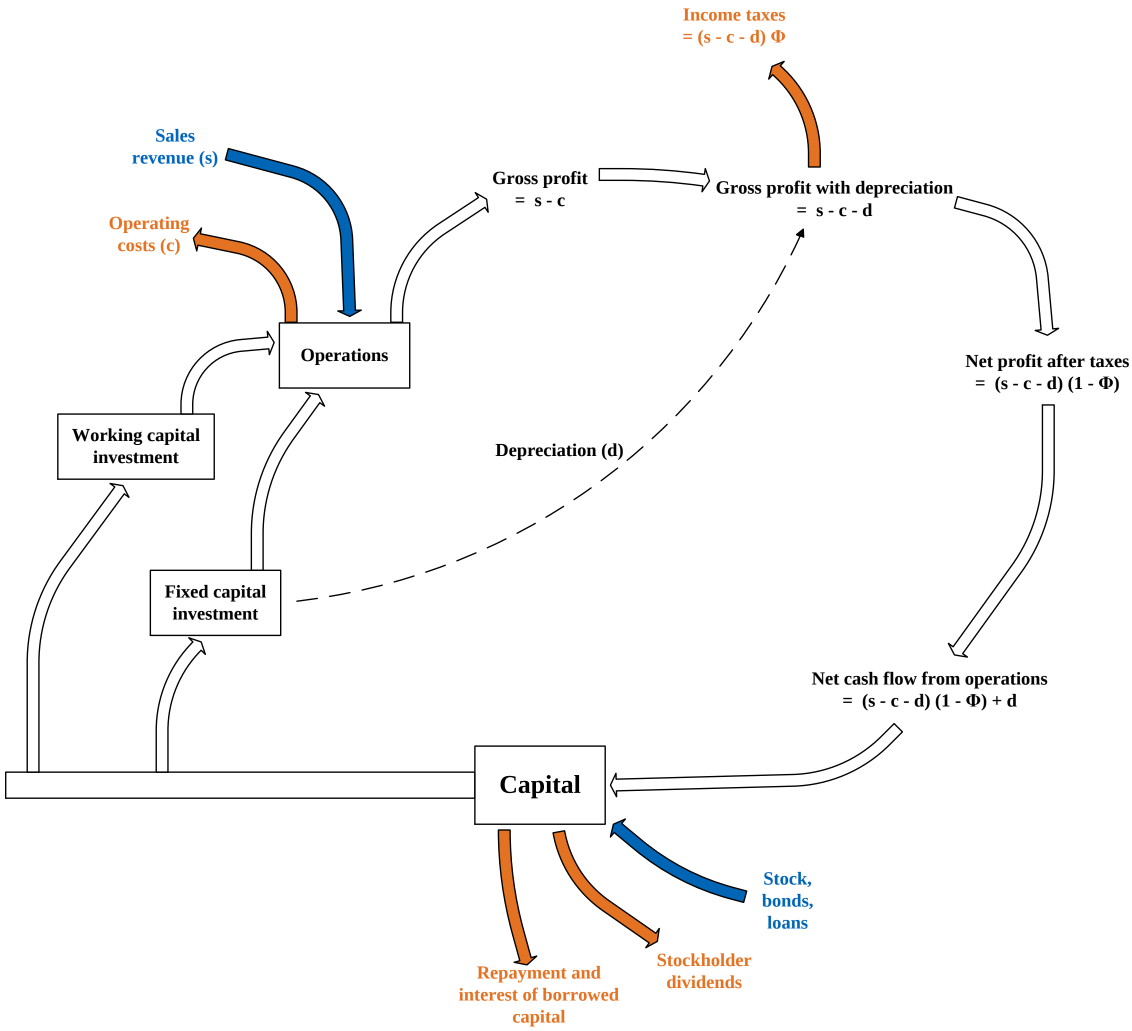


Figure 3: Cash flow for industrial operations based on Peters, Timmerhaus and West (2004).

Profit optimization is an enduring goal, not only during product and process development, but also during operation of existing processes. For this purpose, it is key to understand the numerous cost components involved in chemical production. Below, an introduction to these cost components, as well as their common contribution in the chemical industry compared to other sectors is presented:

– *Raw material*:

  One of the major cost components in chemical production is raw material. Either natural resources or base chemicals serve as the basis in chemical processes. Their share in the overall cost differs strongly depending on the product, but can be dominating, e.g. when precious metals are processed. The contribution of raw materials is twofold, through their purchase price as well as through working capital interest for inventories.

– *Utilities*:

Materials, which are not channelled into the product, but which are necessary to carry out chemical production, are summed up as utilities. A utility which is predominant throughout the entire chemical industry is energy. Steam at pressure levels depending on the required temperature is used for heating chemical reactors or thermal separation processes. Whenever high temperatures are desired, gas, fuel oil or coal is utilised. Electricity is consumed for operating motors of agitators, pumps or compressors. Cooling water is used for heat removal, for instance when exothermal reactions take place. Other utilities include inert gases for equipment purging or catalysts for facilitation of chemical reactions. Although utilities play a role in other sectors as well, their cost share in chemical processes is disproportionately high. They are particularly dominant in processes with extensive use thermal separation units, e.g. in fuel refining.

– *Waste*:

Another cost component, which is disproportionately high in the chemical industry, is the treatment or disposal of waste. Gaseous, liquid or solid by-products are generated during chemical productions. These materials, which in many cases are hazardous, either entail work-up processes or create disposal costs when work-up takes place externally.

– *Packaging and transport*:

As in other sectors, costs are incurred for packaging as well as transportation of the final product. The costs have a higher share when products are hazardous or unstable and special containment is required.

– *Licences*:

In case a chemical is produced based on a process or recipe developed outside the company, licence payments may be incurred. These may either be fixed through the given plant capacity or production volume dependent.

– *Labour*:

Manpower is required for operating chemical plants. Labour includes plant operators, analytics personnel as well as maintenance fitters, electricians and plumbers. Alongside maintenance workers, tools and material for equipment repair add further costs. As most chemical plants are operated 24 h per day, operators often work in shift systems. Labour costs play a minor role in chemical production compared to other sectors. However, they vary strongly dependent on process type. While labour requirements in large scale continuous processes are low, they are comparably high in small scale batch production environments.

– *Investment depreciation*:

  Capital investments, e.g. in production plants, are commonly depreciated over a certain time frame. Depreciation represents capital 'consumption' of the production process. By doing so, invest costs are allocated to product volumes over the life cycle of the plant. Furthermore, depreciation serves as allowance against tax, as income is lessened by annual depreciation before tax is charged. In the heavy chemical industry, depreciation periods between 10 and 15 years are common figures (Heaton 1996). Several strategies for the distribution of the invested capital over the depreciation time frame are deployable, however certain standards are required by local law. Many chemical processes are highly capital intensive. Therefore, depreciation often makes up a mayor share of production costs in the chemical industry. This is especially the case when highly automated continuous processes are applied.

– *Local authority tax and insurance*:

  Chemical plants are also subject to local authority tax and insurance rates. Chemical processes which for instance entail high fire risks result in higher insurance premiums.

– *Overhead*:

  Overhead charges include all other costs which are not allocable to any production process. Overhead for instance covers management, secretarial services, planning and scheduling or research and development. The cost share of overhead is particularly high in the research intensive fine chemical sector, especially when products are only demanded in low volume.

Generally, production cost components can be classified into variable costs, which are assumed to be linearly dependent on volume, as well as fixed costs, whose incurrence is not affected by production volume. For instance, raw material, utilities and waste costs are typically variable and increase with increasing plant utilisation. Plant depreciation and overhead costs on the other hand, are independent of production volume and therefore uplift production costs at low utilisation. Even though classification into variable and fixed costs is a common procedure and also part of cost calculation algorithms in commercial controlling tools for production cost allocation, strict distinction does not represent reality in chemical production. If plants are operated at half of their design capacity, consumed raw materials or utilities may not concurrently drop by 50 %. This is due to the fact that highly customized processing units are designed to function optimally at a certain throughput. Consider for instance a heat exchanger network, in which flow is to be reduced. The flow may become laminar, which worsens the heat transfer and, thereby, increases energy requirements per production volume. Labour costs also lie between zero and linear dependence on production volume. Even though labour requirements for plant operation may decrease with decreasing utilisation, other tasks, such as routine maintenance may remain unaffected. As most cost components entail a less than linear increase with increasing throughput, high plant utilisation is strongly desired in chemical processes, not only for revenue reasons but also for better profitability.

Economies of scale, as originally proposed for the automotive industry by Maxcy and Silberston (1959), is a significant effect in chemical production processes. The Maxcy-Silberston curve, which describes falling unit costs with increasing production scale, is displayed in Figure 4. The major contributor for economies of scale in the chemical industry is capital investment. The effect of scale on investment costs can be estimated with the following non-linear relationship (Heaton 1996):

$$\frac{C_1}{C_2} = \left(\frac{S_1}{S_2}\right)^n \qquad \text{Eq. 2}$$

where C is investment capital, S is plant scale and n is a fractional power.

Common values of n lie between 0.6 and 0.7 (Heaton 1996). Seider et al. (2010) state, the average power is close to 0.6, yielding Eq. 2 the name ‘six-tenth rule’. A detailed list of typical n values for several processing units is presented by Peters, Timmerhaus and West (2004). The importance of economies of scale in the chemical industry has also more recently been emphasized by Jones (2013). There are, however, boundaries for the effectiveness of economies of scale. The fractional power of Eq. 2 may approach or even surpass unity, when for instance equipment becomes to large to be assembled in the manufacturer’s workshop or due to mechanical stability equipment has to be duplicated instead of enlarged.

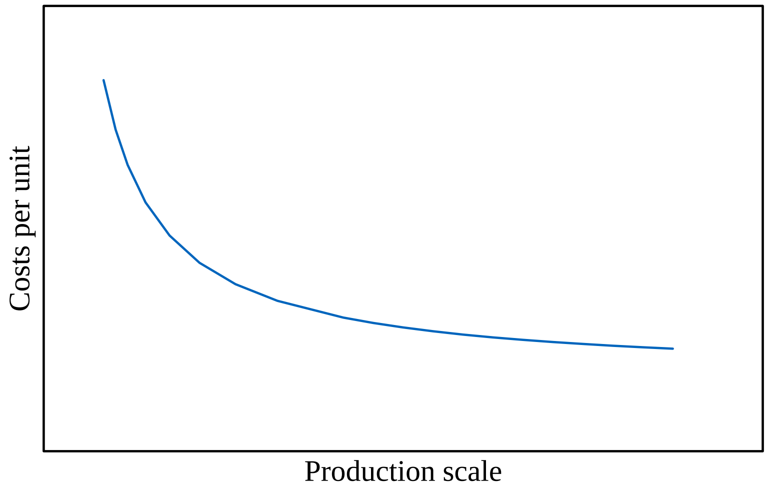


Figure 4: Maxcy-Silberston curve.

2.2 Objectives and strategies for optimization of chemical processes

A top priority of chemical plant design is utilisation of economies of scale to the highest possible extent. However, high design capacity also entails a severe risk whenever volatile markets are served. Due to the fact that most cost components of chemical plant operation are either unaffected by capacity utilisation, or increase in less than linear relation with utilisation, operation below design capacity is highly unfavourable. Furthermore, larger plants commonly entail a longer payback time, and are therefore subject to the risk of unforeseen demand changes in the market. Many chemical plants are therefore designed at conservatively low capacity. As a result, these plants are scheduled to run 24 h per day.

This makes debottlenecking a popular optimization goal during operation of a chemical plant. Whenever market demand exceeds current capacity, companies aspire to enhance their throughput, either through equipment modification or process parameter adjustment of existing equipment. This not only increases revenue, but also in many cases profitability, due to the fact that many cost components do not increase simultaneously. This, however, is not always the case. Many processes for instance run at optimal yield at their design capacity and are sensitive towards throughput deviation in either direction.

The impact of changed utilization on profitability in practice can be derived from a comparison between marginal cost (MC) and average total cost (ATC), defined in Eq. 3

and Eq. 4. MC is defined as additional cost which incurs per additional volume of product. ATC is the specific cost of the overall production volume, which is calculated from fixed cost and MC incurring between zero and produced volume. The point of highest profitability is reached when MC equals ATC.

$$MC = \frac{d\ cost}{d\ volume} \quad \text{Eq. 3}$$

$$ATC = \frac{fixed\ cost}{volume} + \frac{\int_0^{volume} MC\ d\ volume}{volume} \quad \text{Eq. 4}$$

When a process is shifted into a less favourable state, MC tends to increase drastically, since it accounts for increased cost of all output, and not only the incremental cost. The point where MC equals ATC, above which profitability decreases, is often reached rapidly when processes are enhanced above design capacity (see Figure 5 for a schematic example). These considerations show, that throughput increase of an existing plant is a difficult optimization objective, not only because of technical complexity, but also due to potentially drastic effects on profitability.

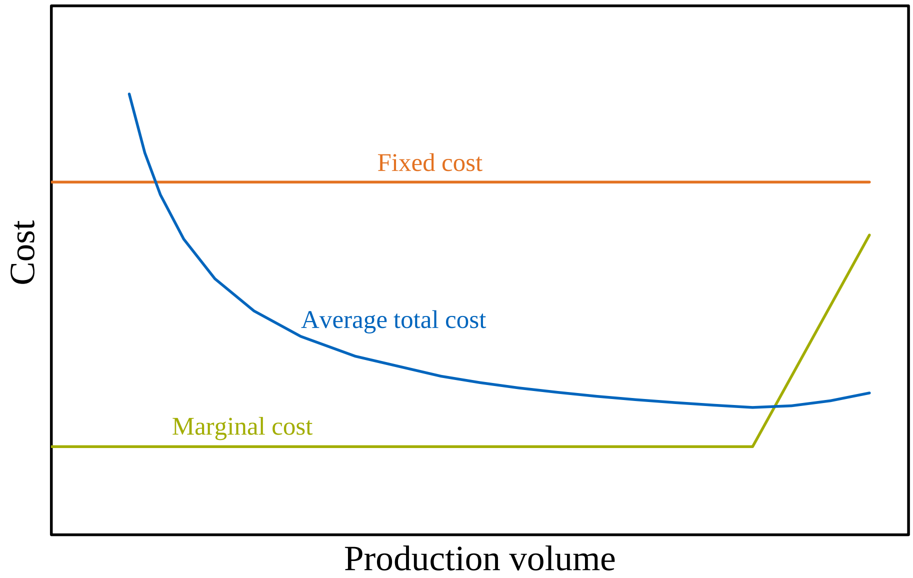


Figure 5: Production costs as a function of throughput.

The concept of MC and ATC is useful for determining whether fulfilling additional orders by increasing capacity increases profitability. In other cases, where capacity exceeds market demand, managing idle time can have high impact on profitability. Production scheduling including product mix, campaign length and batch size decisions potentially affect several cost components. When equipment is under-utilised, even deceleration of process steps may be applied to increase profitability.

A significant lever for improving profitability of chemical production is optimization of the production schedule. In batch production environments, especially in multi purpose plants, optimal scheduling is often approached with mathematical programming strategies. For an introductory example, see Barrera and Evans (1989).

Further optimization objectives of individual cost components are predominantly tackled with technical methods. For instance, focus is put on minimizing energy requirements. Methods, such as pinch technology (Linnhoff and Hindmarsh 1983) aim for heat exchanger networks, which integrate hot and cold streams of a process to an optimum extent. Other methods aspire efficient heat and power integration through heat engines and heat pumps (Colmenares and Seider 1987). Due to the technical complexity of many chemical processes, energy optimization often involves mathematical programming strategies. Minimization of raw material input is also a common objective. Similar to heat exchanger network optimization, methods have been developed to determine minimum use of mass separation agent in complex separation processes (El-Halwagi and Manousiouthakis 1989). Furthermore, yield optimization in chemical reaction systems is a frequent target, which is often tackled with computer aided reaction modelling.

Many of the above outlined optimization approaches have in common, that they utilise computer aided simulation and/or optimization tools. Due to complexity of the system, these sophisticated tools are essential for understanding the technical details and finally optimizing the process.

Recently, the chemical industry has also raised its awareness of statistic process analysis. Through the introduction of Six Sigma initiatives, focus has been set on reducing process variation. Here, a major goal is better utilization of resources, for example of raw material through decreasing scrap rates. For evidence of first successes of Six Sigma in the chemical industry, see Hunter (1999). For an introduction to, as well as a concise literature review of Six Sigma throughout several industries, see Brady and Allen (2006). A profound insight into the Six Sigma methodology is presented by Breyfogle (2003).

2.3 Multi-objective optimization problems

Perhaps more than in any other industry sector, cost components are interrelated in the chemical industry. Modification of a process towards minimization of one cost components may very well cause a shift of other cost components in either direction. For instance a yield increase, which enables more efficient raw material utilisation may be accompanied by higher energy consumption and capacity decrease due to longer batch cycle times. Thus, inevitably trade-offs arise between the individual cost components. These objectives can be integrated into a global optimization goal of cost minimization in a rather straightforward manner. However, there are additional objectives in manufacturing environments, whose integration is more challenging.

Erlach (2010) defined four objective dimensions, which manufacturers in any sector seek to optimize. These dimensions have sub-classes of market objectives and producer objectives. A summary of the dimensions, as well as the respective objectives are shown in Table 2.

Table 2: Objective dimensions in mananufacturing according to Erlach (2010).

Dimension	Producer objectives	Market objectives
Cost effectiveness	High plant utilisation; low production costs; high productivity	Low price
Pace	Low lead time; low inventory	Low delivery time
Quality	Low defect rate	High service level
Variability	-	High ability to fulfil diverse customer requirements

Between the dimensions, a conflict of objectives arises, resulting in a dilemma when optimization is aspired. The term ‘dimensions’ implies that the measures of the objectives are unequal, impeding a mathematical formulation of a global objective function. However, despite this mismatch, all objectives are subordinate to the company goal of gaining profitability. On the one hand, producer objectives mostly directly affect profitability through reduction of cost components. The market objectives on the other hand, indirectly affect profitability, because their fulfilment satisfies customer needs and opens up future business opportunities.

When formulating the global optimization goal, the producer objectives can be directly integrated into an objective function of quantity specific production costs, which is sought to be minimized:

$$min \left\{ \sum \left(\frac{cost}{q_{cc}} \cdot \frac{q_{cc}}{q_p} \right) \right\} \qquad \text{Eq. 5}$$

where q is quantity, subscript cc is cost component and subscript p is product.

Integrating market objectives into the global optimization goal is less tangible, since their impact on profitability is not directly measurable and may only result in delayed benefits. For instance, an improved service level of on time deliveries may lead to additional customer orders in future time. It is, however, highly important to take these objectives into account when optimizing production systems. For this purpose, there are several options available:

- *Conversion to cost components:*
  In order to express the global optimization goal with one objective function, the non-monetary objectives are transformed into cost components. Artificial value is attributed to the fulfilment of market objectives. This, however, requires rather daring predictions on the effect of customer satisfaction on future profit. Even though this option yields a mathematically straightforward formulation of a single objective function, its evaluation may be biased.
- *Pareto efficiency:*
  A concept for solving multi-objective optimization problems is provided through Pareto efficiency. Here, the different optimization dimensions are preserved instead of combined into one objective function. The range of parameter choices is scanned for a smaller set of choices for which no improvement on any objective can be made without worsening the result on any other objective. These choices are labelled Pareto efficient or Pareto front. For instance, if process rearrangements are considered in order to optimize cost and service level, for a Pareto efficient option no parameter variation would be possible which decreases cost and at the same time does not decrease service level. After determination of the Pareto front, decisions can be made based on the diminished set of choices. The Pareto efficiency concept has for instance been utilized when simultaneous economic and environmental optimization was

aspired (Azapagic and Clift 1999, Puigjaner and Guillen-Gosalbez 2008). A brief introduction to Pareto efficiency is presented by Ehrgott (2012).

- *Constrained solution set:*

  Another option for solving multi-objective optimization problems is to set constraints for the objectives which cannot be expressed monetarily. For instance, a service level of 90 % on time deliveries could be set as mandatory, excluding all choices which do not meet this constraint.

2.4 Strategies for solving optimization problems

Above, options have been discussed for integrating different optimization objectives in an objective function. For solving this objective function, the actual process has to be linked to it. There are several options available this purpose:

- *Mathematical programming:*

  Mathematical programming directly integrates process parameters into the objective function. Depending on the formulation, there are several types of mathematical programming. For instance, if the objective function as well as the constraints can be expressed with linear equalities and inequalities, the optimization problem is specified as a linear program. For each type, there are algorithms available, which are capable of determining the global optimum. The Simplex algorithm is the most widely known algorithm for solving linear programs. For an introduction to mathematical programming, see Bradley, Hax, and Magnanti (1977). In the context of chemical process optimization, mathematical programming has been applied to solve batch process scheduling problems. Majozi (2010) provides an introduction to this subject. The advantages of mathematical programming lie in its ability to detect global optima, as well as the low cost of model formulation. However, the system to be optimized has to be represented by an analytical model. Assumptions and simplifications have to be made in case the system is complex and not all aspects are known with certainty. This may result in inadequate representation, a risk which is even elevated, if strong variability is observed in the process.
- *Simulation:*

  If the formulation of an analytical model involves too much uncertainty, the process can be mimicked with a simulation model. Here, instead of an exact mathematical formulation, relations between parameters as found in the real process are modelled without necessarily knowing their physical origin. Simulation models can either be physical or computer based. For computer simulation, there are several types available, which are selected depending on several factors, such as the size and type of the physical system, time dependency or the inclusion of variability. For instance, if large scale manufacturing processes are to be modelled, Discrete Event Simulation is a preferred choice, as it is capable of mimicking time dependent systems including variability. Discrete Event Simulation is introduced in detail in Section 4. Compared to mathematical programming models, simulation models hold the advantage that complex processes can be represented with greater detail. However, since the process is not represented analytically, the process input parameters cannot be integrated into the objective function. Therefore it is not possible to solve the optimization problem analytically. Instead, experiments have to be conducted with the models, in which input parameters are varied and the effect on the objective function is observed. There are several techniques available to reduce the number of experiments necessary to obtain an optimal solution. For example Design Of Experiments (DOE) provides a structured approach to examine the input parameter set for its effect on the objective function. Heuristic procedures such as Evolutionary Algorithms provide directed search within the input parameter set, as the parameters of later experiments are based on evaluation of the objective function of earlier experiments.

– *Experimentation with the real process:*

  A third option for optimization of the objective function is obviously experimentation with the real process. It is the most accurate, but also the most time-consuming and costly option. It may even be impeded in case a parameter change represents capital expenditure, e.g. equipment replacement in a chemical production process. Furthermore, the experimentation may lead to revenue losses if capacity is limited. As with simulation models, it may be an option to reduce the number of experiments required through techniques such as DOE.

Selection of the strategy to solve the optimization problem is accompanied by a trade-off between cost and effort on the one hand and representation detail on the other. The schematic procedure of the three strategies as well as the trade-off is outlined in Figure 6.

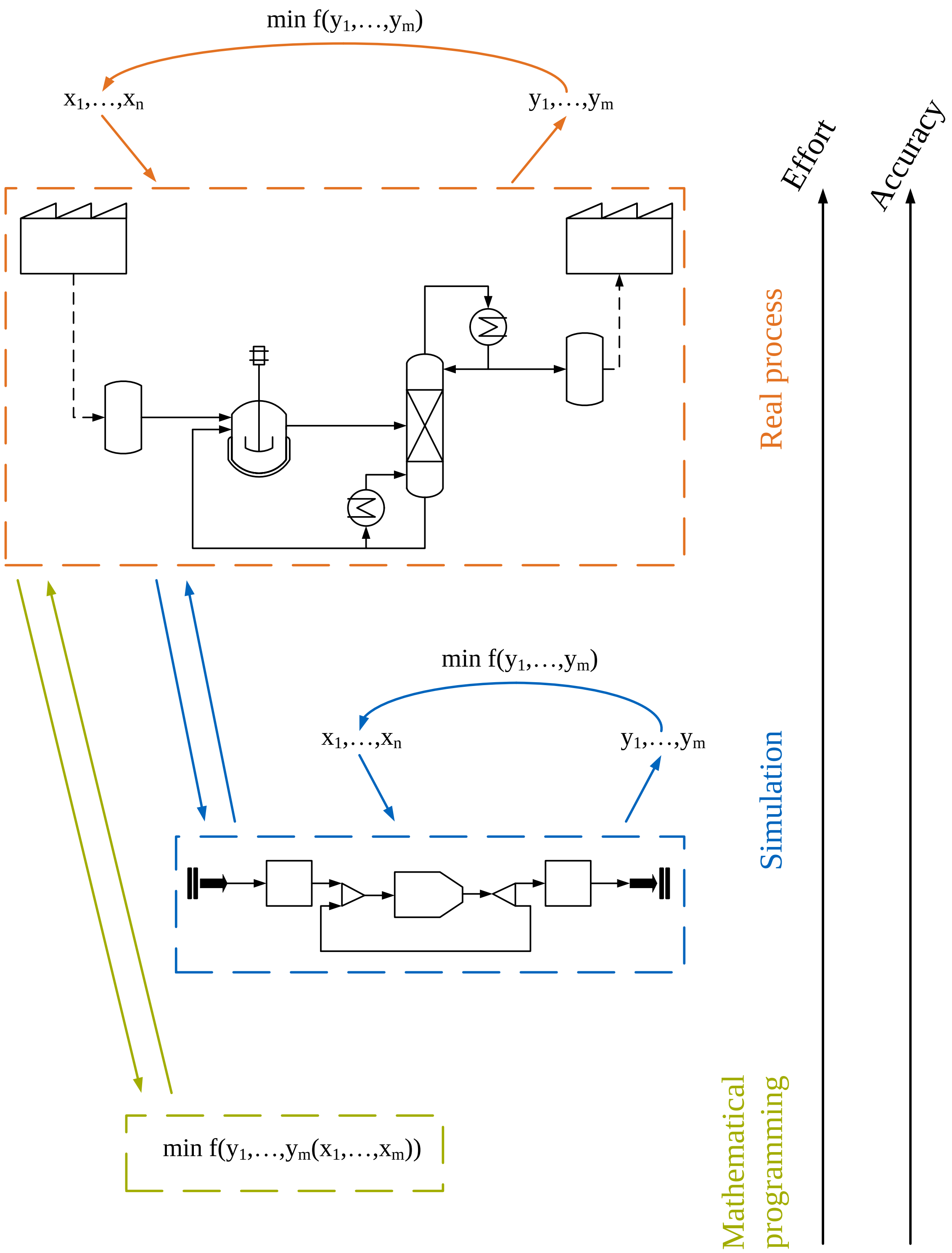


Figure 6: Illustration of options for solving optimization problems.

3 Value Stream Mapping

3.1 VSM – an integral approach to Lean implementation

Effected by the growing interest of western manufacturers in Lean production over the course of the 20th century, researchers, consultants and the companies themselves have developed tools and methods for transforming production environments into a Lean operational state. One widely applied integral method is Value Stream Mapping (VSM), as introduced by Rother and Shook (1999) in the book 'Learning to See'. The authors, who had thoroughly studied the production techniques at Toyota, developed VSM based on the TPS method 'Material and Information Flow Mapping'. VSM is carried out in structured projects. It can be described as "a graphical tool used to map the as-is situation of the organization, to identify opportunities for waste elimination, and to decide the improvements to be implemented to eliminate the waste" (Pavnaskar, Gershenson and Jambekar 2003). The transformation into a Lean operational state is achieved by following several guidelines, which tackle the wastes defined by Ohno (1988). Jones and Womack (2000) describe VSM as 'the simple process of directly observing the flows of information and materials as they now occur, summarizing them visually, and then envisioning a future state with much better performance'.

Erlach (2010) describes VSM as a turbulence avoiding approach to process optimization, as its application leads to definition of clear rules how to steer and operate the process. It entails shortened and well defined lead times and reduced planning efforts. Other approaches on the other hand are rather turbulence controlling, where customer demand is maintained through sophisticated resource planning systems.

Since the development of VSM, its industrial application success has been well documented in the academic literature, primarily focusing on mechanical production processes. For example, Lasa, Laburu, and de Castro Vila (2008) report gainful use of VSM for optimization of a mobile phone parts production process. Seth and Gupta (2005) as well as Singh and Sharma (2009) successfully applied VSM in the Indian automotive industry. Similarly, AR and al-Ashraf (2012) report beneficial VSM deployment at a Malaysian car part supplier. Serrano, Ochoa and de Castro (2008) conducted a broad case study involving six different companies across the manufacturing sector, where VSM was successfully applied and also gaps between theory and practice were identified.

Furthermore, applicability of VSM has also been reported in areas, which deviate from its original field of application, e.g. the wine production industries (Jimenez et al., 2012), the health care sector (Lummus, Vokurka and Rodeghiero 2006) or housing construction (Yu et al. 2009). Seth, Seth and Goel (2008) utilized VSM in a more general project to analyse supply chains of the cotton seed industry.

3.2 Procedure of a VSM project

Rother and Shook (1999) term the entirety of manufacturing and business processes, which contribute to the creation of a product, the Value Stream. In a VSM project, the complete Value Stream is depicted, analysed and improved. A concise introduction to the procedure in a VSM project is presented below. Upon further interest, there are several textbooks available, which cover VSM in great detail. Besides the introductory work by Rother and Shook (1999), more detailed application of VSM has been published on the process level (Rother and Harris 2001) and on the supply chain level (Jones and Womack 2000). A particularly detailed guide to VSM in German language, including multiple examples is provided by Erlach (2010). A different VSM approach, based on several individual tools rather than an integrated project has been introduced by Hines and Rich (1997), its applicability has ben proven by Hines, Rich and Esain (1999).

3.2.1 Selection of a product family

The first step in a VSM project is setting the scope through selection of a product family. Since in many cases production flows of different products are interfering with each other by common resource utilization, they are clustered and analysed in one project. This facilitates deployment of the measures presented below to better understand the Value Stream and detect waste. For the selection, a plant’s products are analysed with the product family matrix, a rather simple tool, which displays processing steps and resources over the products. The products are clustered into families based on similarities in the product family matrix, with emphasis on downstream steps rather than pre-processing steps further upstream. With the selection of a product family a compromise is aspired between an incomplete picture when covering a single product and over-complication when analysing an entire plant. An exemplary product family matrix is shown in Table 3.

Table 3: Exemplary product family matrix.

Product	Process step									Product family
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	
A	x			x		x		x	x	
B	x		x	x		x		x		**1**
C	x		x	x		x		x	x	
D		x	x			x	x			**2**
E		x	x		x	x	x			
F		x		x	x				x	
G	x	x		x	x				x	**3**
H	x	x		x	x				x	

3.2.2 Current state map

With the current state map, the production process of the selected product family is visualized and analysed. This is done interactively with rather simple tools to facilitate participation of everyone involved in the process. Rother and Shook (1999) suggest drawing the current state map while walking along the process and getting information from the plant operators. Commonly the starting point of composing the current state map is the customer end of the process. Thus, the first thing to do is collecting customer requirements. The customer demand per year for each product of the product family is noted down in a data box alongside the factory working days per year (FWD) and the daily labour time (LT). These figures are then converted into the aforementioned takt time (TT), which is also included in the data box:

$$TT = \frac{FWD \cdot LT}{Annual\ demand} \qquad \text{Eq. 6}$$

The current state map comprises production processes and business processes, as well as material flow and information flow. Starting with the customer data box, the current state map is elaborated, following the simple rule that all material flows towards the customer and all information flows away from the customer (see Figure 7).

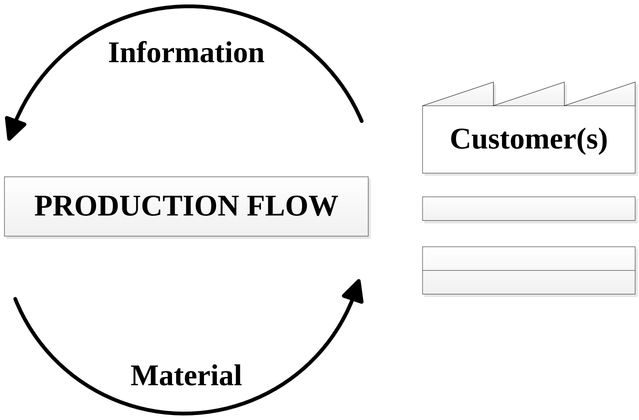


Figure 7: General structure of a VSM.

After determining the customer data, the material processing steps are drawn as boxes, from the supply of raw material over production to final product shipping. The process step boxes are then filled with data while walking ‘through the process’. In order to maintain the customer perspective, data collection is started at the most downstream process step and ends at the most upstream process step. All data should be collected while being present on the shop floor, instead of writing them off of recipes or resource planning systems. Common data included in process step boxes are: the number of operators required for the process step, the number of equivalent equipment/machinery available for the process step; the batch size (BS) of material which is processed simultaneously, the process time (PT) for material from entering to exiting the process step, the cycle time (CT) as the interval between two pieces exiting the process step, the changeover time (COT) which is required for product change on the equipment and the scrap rate. In assembly lines, the data can be acquired simply by counting and stop watch measurements, as the discrete parts being processed are visually tangible.

Between the process steps, the amount of inventory (I) is identified. Again, if discrete parts are processed, this is done visually by counting pieces on the shop floor. Based on this figure, the average residence time as days of inventory (DOI) is determined from the customer demand, utilizing Little’s law (Little 1961):

$$DOI = \frac{I}{Daily\ demand} \quad \text{Eq. 7}$$

An exemplary process step box including the subsequent inventory is presented in Figure 8.

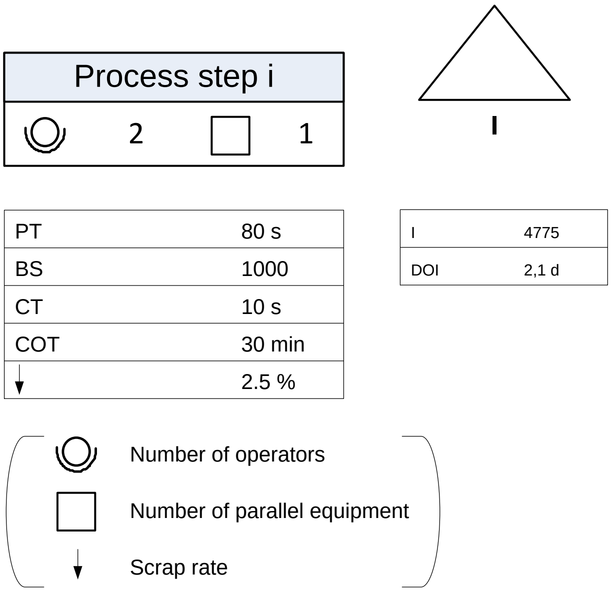


Figure 8: Process step of a VSM current state map.

The next thing to map is the logistics of the process. This includes all information flow between departments involved in steering and operating the process. The information flow is depicted with arrows from the source to the receiver. For instance, information about incoming product orders could flow from the customer to the sales department, which passes information about processing orders to the production control department. The production control department subsequently schedules the production shop floor by sending information to specific production process steps. In order to be more specific, data boxes including the type and frequency of information flow are added to the arrows. Electronically transmitted information flow is represented by lightening-like arrows. By mapping the information flow, a clear picture is gained about the nature of material flow. When it is known, which process steps are scheduled, it becomes obvious, how material flows between the process steps. Material is commonly pushed towards the customer downstream of the scheduled process step. This is indicated by a stripped arrow. A rather simple current state map filled with process logistics is displayed in Figure 9.

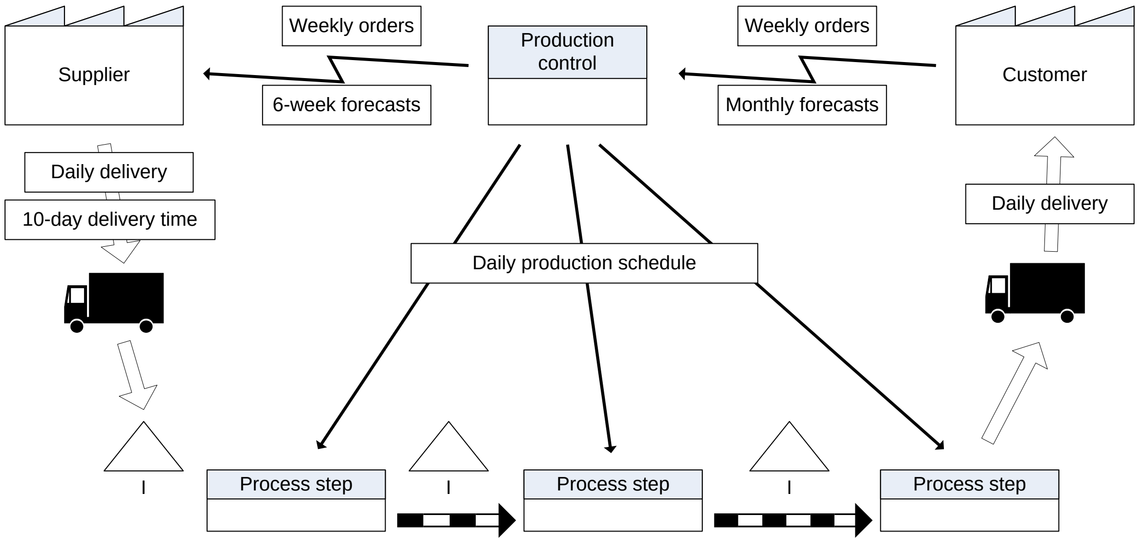


Figure 9: Exemplary VSM current state map including process logistics.

After completion of the current state map, the process performance according to Lean measures is determined. This is commonly done by calculation of the following characteristic numbers:

– *Process lead time (PLT):*
  The process lead time of a production process can be described as the residence time of material from entering to leaving the process, which in a VSM commonly comprises all operations within the production site from raw material receipt to final product shipping. PLT is obtained from DOI between process steps, as well the work in process (WIP) within the process steps. This leads to the following calculation:

$$PLT = \sum_{Step\ 1}^{Step\ n} \frac{WIP}{Daily\ demand} + \sum_{Inventory\ 1}^{Inventory\ m} DOI \qquad \text{Eq. 8}$$

– *Flow ratio (FR):*
  An essential key figure for evaluating the implementation of Lean production is the flow ratio. It shows the ratio between processing time, in this context also connoted value added time, and the PLT:

$$FR = \frac{\sum_{Step\ 1}^{Step\ n} PT}{PLT} \qquad \text{Eq. 9}$$

The process performance is also visualized in the current state map. For this purpose, a time line is included below the map, where for each process step PT and DOI and for each inventory DOI is entered (see Figure 10).

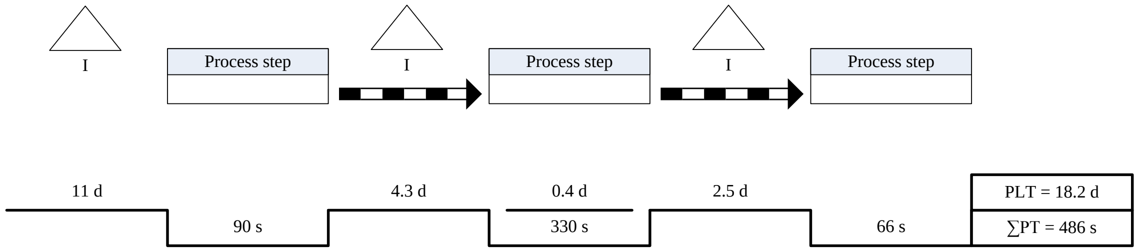


Figure 10: Timeline of a VSM current state map.

The current state is further evaluated with the operator balance chart, a bar chart in which the cycle time of each process is compared to the takt time demanded by the customer. As synchronisation of all process steps with the takt time is aspired in Lean production, the operator balance chart visualizes deficiencies, be it bottlenecks in case of cycle times above the takt time or overdimensioned process steps with cycle times markedly below the takt time. An exemplary operator balance chart is displayed in Figure 11.

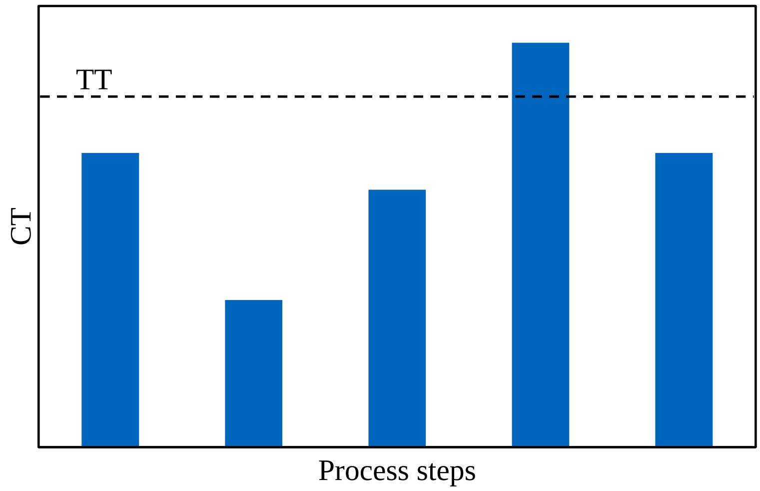


Figure 11: Exemplary operator balance chart.

3.2.3 Future state map

After completion of the current state map, modifications towards a Lean production process are evaluated. To begin with, these modifications focus on the rearrangement of the process, without reassessing product design, process technology or plant location. Rother and Shook (1999, p. 49) suggest to think 'What can we do with what we have?'.

This rearrangement is achieved in a structured way by elaborating the future state map. Rother and Shook (1999) propose a set of guidelines, which facility reduction of the seven wastes (Ohno 1988), with overproduction predominantly being tackled:

– *Guideline #1 – Produce to your takt time:*
  All individual process steps should be oriented towards the takt time demanded by the customer. By doing so, the pace of production is synchronized with the pace of sales. It is a central element for avoiding overproduction.
– *Guideline #2 – Develop continuous flow wherever possible:*
  Consecutive process steps should be integrated into areas of continuous flow whenever possible. Process steps which cannot be integrated should be coupled with first in first out (FIFO) flow and strict accumulation limit. By following guideline 2, several wastes are reduced. For instance excess transport is avoided and the build-up of inventory is constricted, consequently lowering the risk of overproduction.
– *Guideline #3 – Use supermarkets to control production where continuous flow does not extend upstream:*
  Whenever two consecutive process steps cannot be coupled, e.g. because cycle times differ too much or the steps are spatially separated, processing decoupled from the customer is avoided through application of material pull systems. Instead of scheduling process steps individually, the operations on the shop floor are organized through self-regulation. The downstream 'customer' process step orders material from the upstream 'supplier' process step according to its own demand. In order to avoid idling of the customer process step, the pull system is buffered with a supermarket with limited capacity (see Figure 12). Initiated by an order of material from the customer process step, commonly placed on a so-called withdrawal Kanban card, a material handler withdraws the required material from the supermarket. The withdrawal subsequently causes the release of a production Kanban sent to the supplier process step, which then produces

the material to replenish the supermarket. Apart from this Kanban supermarket system, there are several other options to establish pull. For an introduction to pull systems, see Monden (1981), Rother and Shook (1999) or Erlach (2010). Hopp and Spearman (2008) provide more detailed analysis on pull systems as well as their performance.

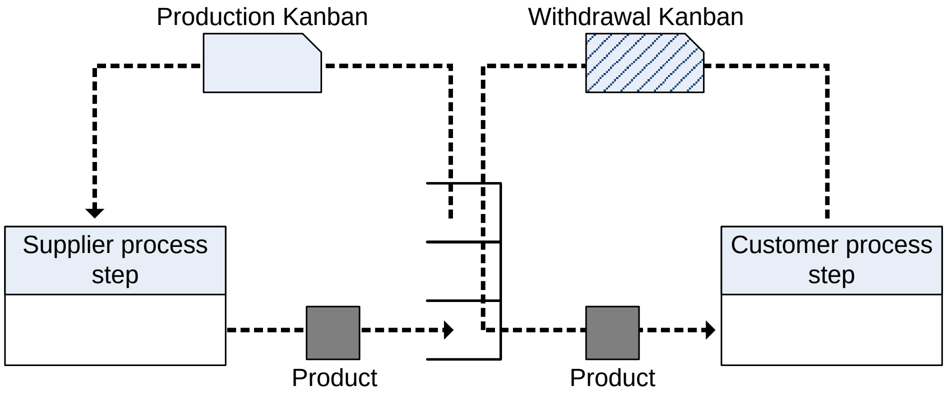


Figure 12: Demonstration of a supermarket pull system.

– *Guideline #4 – Try to send the customer schedule to only one production process step:*

  A key result of establishing continuous flow and material pull throughout the process is self-regulation. This leads to scheduling necessity at only one process step, which is called the pacemaker. Upstream of the pacemaker, material is pulled and downstream of the pacemaker flows continuously towards the customer (see Figure 13). Ideally, scheduling at the pacemaker is synchronized with the takt time. The pacemaker concept is closely related to, but not to be confused with the theory of constraints and the drum buffer rope concept developed by Goldratt (Goldratt and Cox 1992).

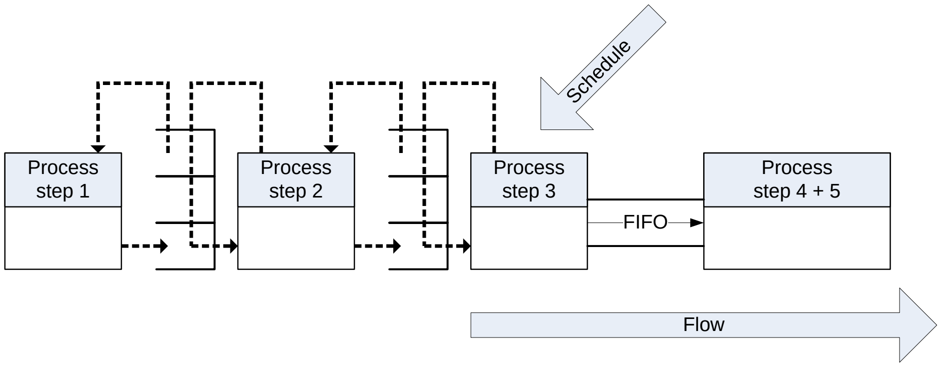


Figure 13: Scheduling at the pacemaker process step.

- *Guideline #5 – Distribute the production of different products evenly over time at the pacemaker process step. (Level the production mix):*

  Instead of long runs of single products, for the future state map even distribution of all products over time is aspired. Rother and Shook (1999) state, that at the expense of more frequent changeovers, this leads to quicker response to customer requirements with short lead time while holding little finished goods inventory.
- *Guideline #6 – Create an "initial pull" by releasing and withdrawing small, consistent increments of work at the pacemaker process step. (Level the production volume):*

  Furthermore, the work should be released to the pacemaker in equal and small as possible volumes. In order to avoid build-up of inventory within the process, work is only released to the pacemaker when an equal quantity of final product is withdrawn from the process. This concept is called "initial pull".
- *Guideline #7 – Develop the ability to make "every part every day" (then every shift, then every hour or pallet or pitch) in fabrication process steps upstream of the pacemaker process:*

  Guideline #5 and guideline #6 facilitate the ability to respond quickly to customer demand changes. Small increments of orders for different products are spread evenly over time. In order to measure the success of this achievement, the key figure "every part every interval" (EPEx) is introduced. It indicates the time interval within which the process changes over to produce all product variations and should be as low as possible.

Rother and Shook (1999) provide a sequence of questions for VSM practitioners to ask in order to develop the future state systematically. The questions are formulated to support utilization of the guidelines presented above. The final question asks which process improvements are necessary to implement the future state. These improvements could include changeover time reduction, increase of uptime or redistribution of the operators among the process steps. Asking for process improvements is on purpose the last element of future state mapping, making it subordinate to development of the Lean value stream.

3.2.4 Work plan for achieving the future state

After the future state map has been compiled, a work plan for its implementation is set up. Since the future state map often suggests changes to the overall production process within a plant, implementation is a complex procedure. Therefore it is recommended to break implementation into so-called value stream loops, which cover a certain set of process steps and to deal with them consecutively. The first loop for example could be the pacemaker loop, which comprises selection of the pacemaker process steps and establishing of continuous flow for all downstream process steps towards the customer. This loop is rather independent of upstream flow and could be implemented exclusively. The introduction of material pull upstream of the pacemaker could be faced with the second value stream loop. Integration of raw material into the pull system could be subject of the third value stream loop. Rother and Shook (1999) also emphasize the importance to manage implementation of the future state, including timelines, checkpoints and measurable goals.

3.3 VSM in the context of optimization

VSM provides a framework for establishing Lean production and therefore, when applied, can positively impact the economic performance of a production facility. However, quantification of the benefit is a difficult challenge. This is mainly due to the fact that some actions do not directly influence cost components, but have a delayed impact. Womack and Jones (1996) state that Lean manufacturing is not a panacea to solve short term competitive problems and that its effects can only be seen in the long term. Apart from direct monetary effects, VSM implementation potentially facilitates improvements on market objectives as defined by Erlach (2010). Furthermore, it leads to exposure of weaknesses in the process, generating momentum to increase satisfaction of producer objectives.

Several approaches have been published on measuring the performance and success of Lean and VSM implementation. Karlsson and Åhlström (1996) proposed nine parameters according to which the change towards Lean production can be assessed:

- Elimination of waste
- Continuous improvement
- Zero defects
- Just In Time
- Pull instead of push
- Multifunctional teams
- Decentralized responsibilities
- Integration of functions
- Vertical information systems

Evaluation of these parameters is carried out in a rather qualitative way. Chauhan and Singh (2012) conducted a survey among Indian manufacturing firms, which rated their perceived status of fulfilment of these parameters. A similar survey in the UK ceramics tableware industry is presented by Soriano-Meier and Forrester (2002). Rivera and Chen (2007) provide a quantitative approach, but only focus on direct costs through cost time profiles. A more holistic approach for assessing the impact of VSM is presented by Sihn and Pfeffer (2013). Besides monetary benefits, as well as costs of VSM implementation, they include the non-monetary objectives FR, EPEx, overall equipment effectiveness (OEE) and space, which they normalise and couple in an objective function. Through these evaluations, they assess different potential future state in order to select the most beneficial.

Even though evaluation of Lean and VSM implementation is quite present in academic literature, potential trade-offs have not been considered quantitatively to date. Most approaches are based on the question ‘to what degree has our process been transformed into a Lean state?’, rather than ‘how beneficial is the Lean state?’. The positive impact of Lean implementation is accepted as a given fact. On the one hand, this may be due to the challenges to grasp the benefits of Lean production presented above. On the other hand, a legitimate common understanding has been established about Lean being the superior production technique (see Section 1.1).

However, especially when the application of VSM is aspired in sectors which differ from its original field of application, e.g. in the chemical industry, positive impact cannot be taken for granted (see Section 1.3). For evaluating the benefit of VSM, it is valuable to formulate a multi-objective optimization problem. This requires a closer look at the benefit mechanisms of VSM. These can be categorized into direct benefits on producer objectives, delayed benefits on producer objectives and benefits on market objectives (see Figure 14).

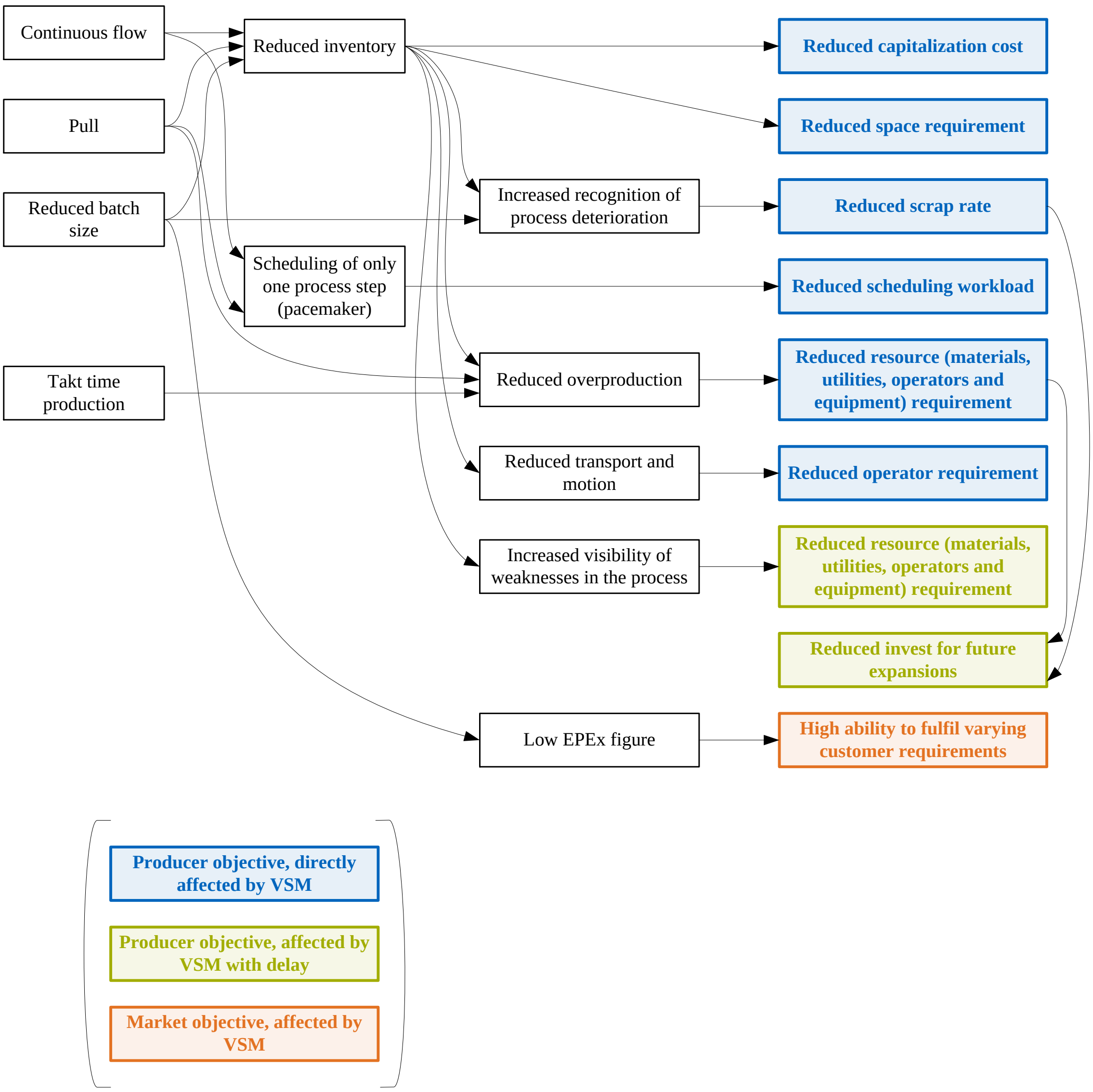


Figure 14: Benefits and underlying mechanisms of VSM.

The benefits on direct producer objectives can be related to cost components in a rather straightforward manner in order to formulate an objective function. Integration of delayed benefits on producer objectives as well as benefits on market objectives into the objective function proves to be more difficult, because their influence on cost components is not directly measurable. Here, assumptions have to be made potentially based on best practice experience. On the other hand, negligence of these benefits leads to more conservative analysis.

3.4 VSM for chemical process optimization

3.4.1 Limitations

Coverage of VSM applied to chemical processes in the academic literature is rather narrow. The only VSM study in chemical production is presented by Anvar and Irannejad (2010). They emphasize that time is the central factor considered in VSM, however other factors such as energy consumption are more important in many chemical processes and should therefore be integrated into the method. Successful VSM application has been reported in industries outlined as the process sector which are to some extent similar to the chemical industry. For instance studies in the steel industry (Abdulmalek and Rajgopal 2006) and the wine producing industries (Jimenez et al. 2012) have been published. King (2009) includes VSM as a central tool in a textbook on Lean implementation in the process sector.

Several limitations of VSM can be found when applying the method to chemical processes, which presumably lead to its rather scarce deployment in the sector. These limitations can roughly be structured into shortcomings of analysis, constraints and trade-offs. They are all related to features that are predominantly, but not exclusively, existent in the chemical industry.

– *Shortcomings of analysis:*
  A major strength of VSM is the simplicity with which processes are visualised and analysed. The simple maps and the straightforward calculations allow participation of everyone involved in the process. In chemical processes however, material flow can be highly complex and non-linear. Features such as recycling, merging and diverging of material flow make the mapping approach

much more difficult than in assembly lines. For the current state map, material flow is determined by material counting and time measurements with a stopwatch while walking through the shop floor. In chemical processes this is often not possible, because material flow is subject to complicated mass balances. Furthermore, in contrast to discrete part manufacturing, chemical flow is often not visible, because it takes place in pipelines and closed tanks.

Another shortcoming of VSM is its lacking inclusion of process dynamics. Many production plants, not only in the chemical industry, are subject to heavy variability of the process itself as well as the customer demand. When gathering data for the current state map while walking through the process, a rather static picture is developed. Consequently, the variability of the operating conditions may not be fully accounted for and in the worst case a poorly performing future state may be developed.

– *Constraints:*

  VSM future state guidelines aim to facilitate process rearrangement without major capital investment. In chemical processes, this is often not possible. Apart from multipurpose batch plants, chemical plants are commonly linked with permanently mounted pipelines dedicated to single products or product families. Furthermore, equipment in the chemical industry is commonly large and integrated into a utility supply network, making relocation without larger investment difficult or even impossible. If equipment is dedicated to a single purpose, options to restructure the process are even more limited.

  Due to the fact that chemical production is rather capital intensive than labour intensive, flow is often constrained by equipment, which is scheduled to operate 24 h per day. Thus, levelling the throughput of the process steps and synchronising them with the takt time through shifting the operator workload may not be possible.

  Moreover, the diverging flow pattern from few raw materials to a wide variety of final products of many chemical processes makes establishing initial pull far more complicated.

– *Trade-offs:*

  VSM future state guidelines #5, #6 and #7 promote increased numbers of changeovers and batch size reduction in order to facilitate the highest possible flow degree. In assembly line processes, changeovers merely cause time efforts, for instance for exchanging the tools of a machine. These time efforts may even be reduced through application of SMED. In chemical processes on the other hand, changeovers additionally entail time for cleaning the equipment to avoid cross-contamination and time to stabilise the desired process parameters. These efforts often entail excess wastewater production, increased consumption of utilities and reduced yield (see Table 4). Thus, inevitably trade-offs emerge between VSM benefits and optimization goals for various cost components. The risk that VSM does not yield a cost optimized state is even amplified because these cost components often contribute heavily to the overall production costs of chemical processes.

Batch size reduction may also cause severe time efforts and impact cost components negatively in chemical processes. This is mainly due to the fact that batching occurs differently in many chemical processes compared to assembly lines. In assembly lines the batch size is determined by the amount material of the same kind that piles up in front of the process step before it is processed piece after piece. In chemical batch processes on the other hand, batching actually takes place within the process step, where material is processed simultaneously. This causes the process time to be a less than linear function of the batch size (Koulouris, Calandranis and Petrides 2000). As the worst case, both figures are often independent of each other. This means, that halving of the batch size potentially leads to doubling of the cycle time and halving of the capacity. Moreover, process equipment is often designed to operate at a certain batch size at its economic optimum. Thus, for instance specific energy consumption may increase in case of batch size reduction.

Table 4: Effects of changeovers for selected process types (general trends, qualitative).

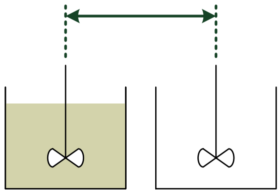
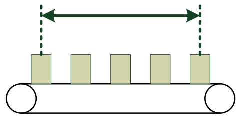
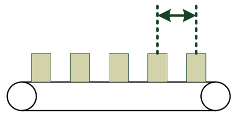
	Mounting	Coating	Heat treating	Mixing	Chemical reacting	Thermal separation	Mechanical separation
Assembly line process	Yes	Yes	Yes	No	No	No	No
Chemical process	No	Yes	Yes	Yes	Yes	Yes	Yes
Energy consumption	0	+	++	+	++	++	+
Raw material consumption	0	+	0	+	++	+	+
Water/cleaning agent consumption	+	+	+	++	++	+	+
Manpower	+	+	+	+	+	+	+
Capacity	-	-	-	--	--	--	--
Cross-contamination risk	0	+	0	+	+	+	+

3.4.2 Potential adaptions

While the constraints have to be accepted, reduction of the shortcomings of analysis as well as evaluation of the trade-offs can be achieved through enhancement of VSM with further tools. However, in order to maintain the strengths of VSM originating in the simplicity of the method which allows straightforward involvement of all process experts, it is advisable to add sophisticated tools decoupled from the original procedure.

When adapting VSM to chemical processes, first of all, several measures need to be adjusted in order to map the process adequately. In Table 5, a suggestion is made for the definition of time measures of chemical batch and continuous process steps.

Table 5: VSM measures adjusted for chemical batch and continuous process steps.

Measure	Batch process	Continuous process	Unit
Process Time (PT)			s
Cycle Time (CT)	BT / BS		s kg^{-1} or s piece^{-1}
Batch Time (BT)	PT	PT + CT * BS	s

For the changeover time, more detailed information may be required. Mapping of contributions to all cost components during changeover is mandatory to capture trade-offs. These could for example include energy consumption, wastewater production or material losses. The changeover time could also be separated into cleaning time, start-up time and equilibration time in order to gain a better understanding.

For the steady state processing phase, it is also valuable to include details on the consumption of energy and other utilities. Moreover, as material flow is rarely linear in chemical processes, the material balance must be determined in order to relate measures to the output at the customer end of the process. Both, the cycle time and the days of inventory are quantity related figures, which have to be scaled to the product quantity for further analysis. This can be done with the introduction of a mass correction factor f, derived from the material balance. For each process step (see Figure 15 for clarification), f is determined as:

$$f_i = \frac{q_i}{q_{i-1}} \qquad \text{Eq. 10}$$

In order to determine the product related cycle time and the correct days of inventory, the following calculations apply:

$$CT_i = \frac{t_i}{q_i}\left(\prod_{k=i+1}^{n} f_k\right)^{-1} \qquad \text{Eq. 11}$$

$$DOI_i = \frac{q_i|_{I_i}}{\left.\frac{q_n}{t}\right|_{cutomer}} \left(\prod_{k=i+1}^{n} f_k \right) \qquad \text{Eq. 12}$$

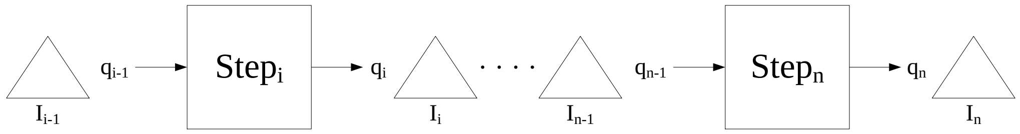


Figure 15: Illustration of process steps for VSM measure adjustments.

Many of these data may not be directly available, and therefore require analysis of process control systems and/or heat and mass balances. Utilization of these tools may also be helpful to check whether the current state map captures the process routing correctly. However these additional efforts necessitate the involvement of process engineering experts, unlike in assembly line production, where process flow can be observed directly on the shop floor.

4 Discrete Event Simulation for decision support in complex environments

The adaptions of VSM to chemical processes introduced in the previous section enable the creation of a more precise current state map, which accounts for complex mass balances and includes information on relevant cost components potentially causing trade-offs. However, several other limitations remain when creating the future state map. The original VSM approach is not able to indicate whether the proposed future state is feasible by meeting the customer demand and whether it is beneficial after consideration of all cost components affected by rearrangement of the process. Without addressing these issues after creation of a future state map, implementation can become a costly iterative procedure. Furthermore, it is crucial to assure and quantify benefits of any improvement project for gaining management support and approval for implementation.

The limitations are mainly rooted in process complexity, which hand-drawn maps are unable to capture. For overcoming them, Discrete Event Simulation (DES) is a very promising add-on. The method is capable modelling complex process sequences including variability in great detail. In the following section, first the functionality and capability of DES is introduced briefly. Subsequently, a literature review of its deployment in the context of VSM is presented. Then, advancements of DES towards its application in chemical processes are discussed and a DES integrated VSM method for chemical processes is elaborated. Finally, further application of DES for chemical process optimization beyond VSM is considered.

4.1 Introduction to DES

Simulation is a frequently applied tool in chemical engineering. With the aid of simulation, for instance complex chemical reactions, fluid flow within reactors or thermal separation processes are explored. These types of simulation are commonly based on numeric evaluation of physical and/or chemical laws and attributes. The attributes of the modelled system change continuously over time. The simulation model is therefore normally solved continuously, or more precisely speaking, at infinitesimally small, equidistant time steps.

The main difference between DES and the above outlined concept of simulation is its evaluation over time. The state of DES models does not change at equidistant time steps, but at discrete points with varying time intervals in between. DES models commonly comprise a system of *entities* with certain *attributes*. With the occurrence of an *event*, *activities* are initiated, which effect an attribute change. In a DES model of a discrete parts manufacturing plant for instance, an entity could be a part, an attribute of the part could be its status changing from raw material to final product over time, an event could be the part entering a machining process and an activity could be the machining process itself. DES models are also commonly, but not necessarily, stochastic and therefore non-deterministic. Probability distributions of processes observed in the real system are often integrated into the model in order to facilitate a more adequate representation. Figure 16 shows a classification scheme for simulation models. Most Discrete Event Simulation models can be best described as stochastic due to the involvement of randomness, dynamic due to the model's evolution over time and discrete due to state changes at discrete points in time.

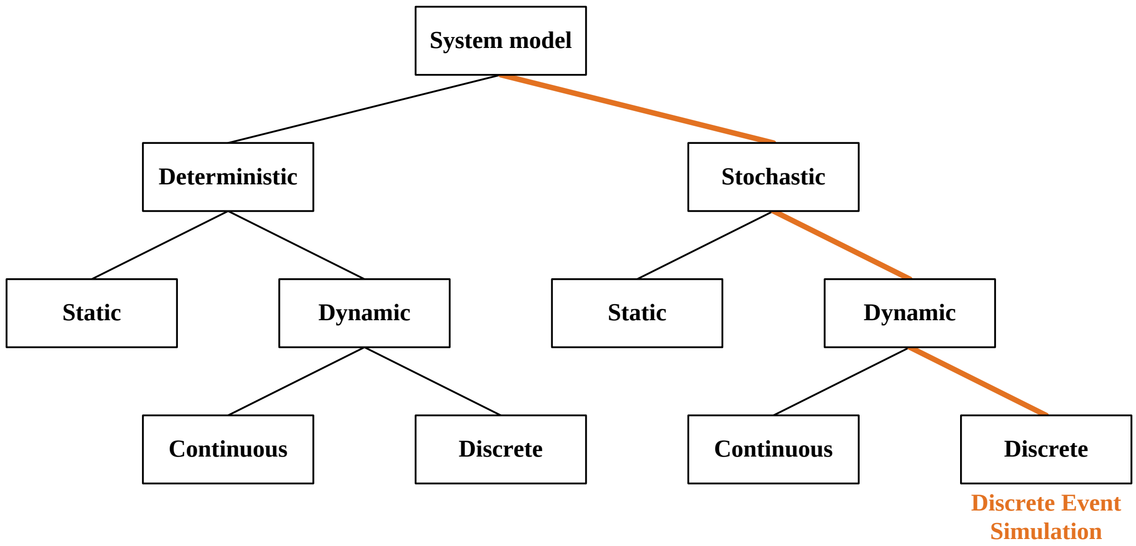


Figure 16: Classification scheme for simulation models (Leemis and Park 2006).

Typical fields of application of DES are logistics and supply chains, transportation and traffic or health care facilities. It is also widely used for modelling discrete part manufacturing systems, for example to determine capacity. Detailed information about the application fields of DES is provided by Bangsow (2012). For an introductory example of a DES model, cf. White and Ingalls (2009). Upon further interest in the functionality of DES, see the simulation textbooks by Banks (1998), Banks et al. (2009) or Law (2007).

4.2 Steps in a DES study

For successful application, DES studies are commonly structured into several steps (see Figure 17). Below, this process is briefly introduced. In the interest of clarity, it is structured into four sections, as indicated in the figure.

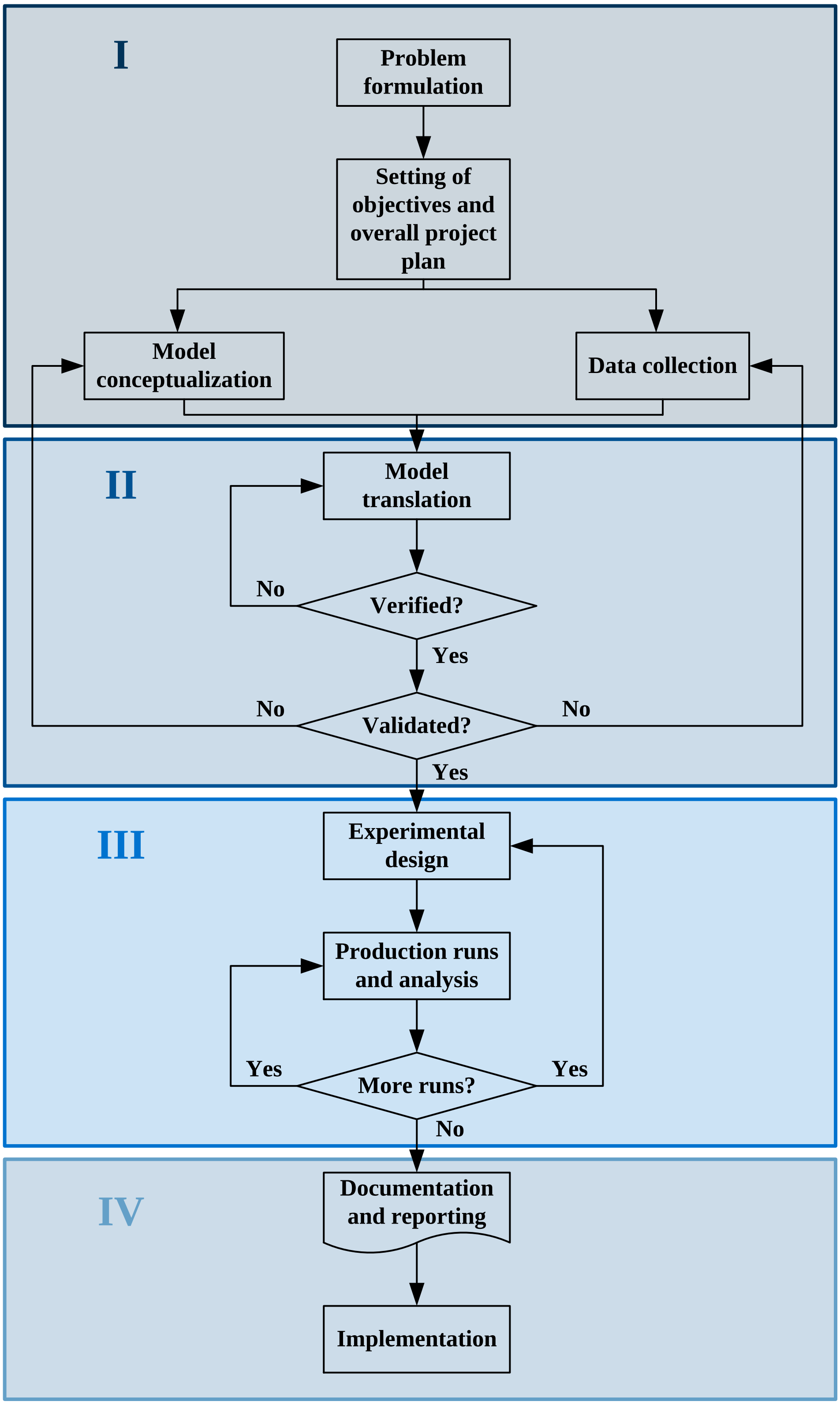


Figure 17: Steps in a DES study (Banks et al. 2009).

– *Section I:*

Section I contains preliminary steps prior to the actual modelling. In the first steps ‘problem formulation’ and ‘setting of objectives and overall project plan’, a common understanding of problem and goal is created and the project is scoped. These steps should also determine whether DES simulation is the appropriate tool to solve the problem. Consecutively, the model is conceptualized. The conceptual model, also frequently called assumptions document, is a document which is composed in order to find an appropriate abstraction level for the simulation model. Here, decisions are made what to include in the simulation model. A one-to-one mapping of the real process unnecessarily raises modelling cost and elevates error risks. Therefore it is highly important to determine the essential features of the system prior to implementation in the simulation model. Law (2007) advises to involve Subject Matter Experts (SMEs) of the real process in determining abstraction level. Conceptual models commonly contain the goal and specific issues to be addressed, a process flow diagram, detailed description of subsystems, simplifying assumptions and their reasons, limitations of the model, data set summaries for model input parameters as well as sources of important information (Law 2007). For detailed information on model conceptualization, see Robinson (2004). In parallel to formulating the conceptual model, data collection is initiated. Data collection is crucial for model validity and commonly accounts for a significant time share of a DES project. DES models usually embrace randomness of the real system and therefore require significant sets of data. When modelling manufacturing systems, these data may include processing times, time between machine failures or machine repair times. Based on the collected data for input random variables, if possible, a probability distribution is selected to incorporate the variable into the simulation model. For an introduction to various probability distributions of both discrete and continuous type which are suited to simulation input modelling, see Law (2007). Fitting the parameters of a theoretical distribution to observed data is commonly performed with the maximum likelihood method or the method of moments (Law 2007). For determining how well the fitted distribution represents the input or process variable, there are several hypothesis tests available, such as the

Anderson-Darling test (Anderson and Darling 1954) or the Kolmogorov-Smirnov test (Massey Jr 1951).

A prerequisite for the validity of distribution fitting is that the data are independent and identically distributed (IID), which means that each data point is independent of the others and that all data points are drawn from identical distributions. In chemical processes, many parameters are autocorreleted and, thus, not independent. Consider for example a chemical reaction in a batch reactor without temperature control, where reaction kinetics depend on ambient temperature. Just as the temperature, the reaction time will almost certainly be autocorrelated, essentially meaning that a slow batch is likely to be followed by another slow batch. The presence of autocorrelation can have major impact on the results and, thus, the validity of simulation models (Livny, Melamed and Tsiolis 1993). There are several options available to model autoregression of continuous data, such as Standard Autoregressive or Autoregressive Moving-Average (Box, Jenkins and Reinsel 2008).

– *Section II:*

Section II comprises translation of the conceptual model into the actual DES model as well as verification and validation of the DES model. Even though DES can be performed with programming languages, commonly special purpose software packages are used. Pre-programmed algorithms for generally required features, such as advancing the simulation time or determining the next event for changing the state of the model reduce the modelling efforts. Contemporary DES packages provide a graphical modelling interface, limiting the programming requirement for the modeller to a minimum extent. The model is commonly synthesized as a flow-sheet-like structure of pre-defined blocks representing for instance queues or activities (see Figure 18 for an exemplary model built with the DES package ExtendSim®). An overview over available simulation packages tailored to a multitude of applications is provided regularly by the scientific journal *OR/MS Today*, see for instance Swain (2013).

Figure 18: Simple DES model implemented in ExtendSim®[1].

After translation of the conceptual model into the simulation model, it is essential to check whether the model is an accurate representation of the actual system and, ultimately, correct conclusions are drawn from experimentation with the model. Therefore, the model has to be verified, i.e. is the conceptual model translated correctly into the simulation model? – and validated, i.e. does the simulation model behave in the same way as the real system? For a logical overview of how verification and validation is integrated in the modelling process, see Figure 19. There are several tools and methods available for verification and validation, see for instance Sargent (2013).

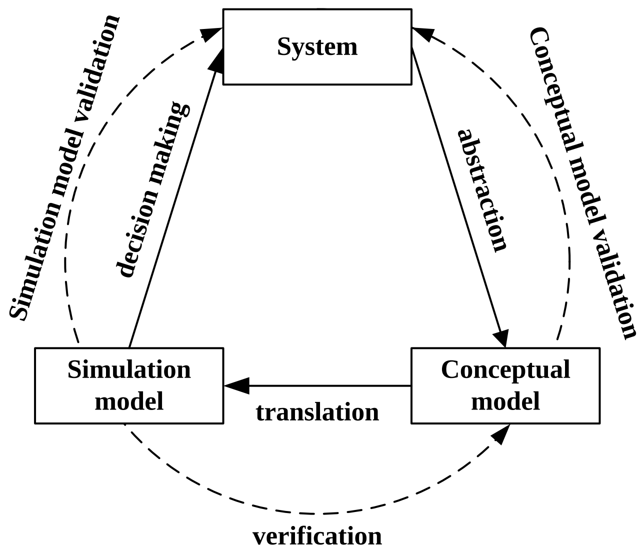


Figure 19: Elements of the DES modelling process.

– *Section III:*

After proving validity of the DES model, experiments can be designed, planned and conducted. When a multitude of system settings is under consideration, it is

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advisable to apply either experimental design or optimum-seeking heuristics in order to reduce the number of simulation runs. For an introduction to the application of experimental design with simulation models, see Kleijnen et al. (2005). Carson and Maria (1997) provide an overview of heuristic optimum-seeking methods applied to simulation models, such as Genetic Algorithms, Evolutionary Strategies, Simulated Annealing or Tabu Search.

As DES models are commonly non-deterministic with random input parameters, one simulation run results only in one data point of an unknown probability distribution. Thus, the mean result has to be estimated from multiple observations:

$$\mu = \bar{X} \pm t_{n-1,1-\alpha/2}\sqrt{\frac{S^2}{n}} \qquad \text{Eq. 13}$$

where μ is the real mean, $\overline{X}$ is the observed mean, t is the t-distribution value, n is the number of observations, α is the confidence level and S is the observed standard deviation.

These observations need to be IID, which is commonly not the case when they are drawn from a single simulation run, like for instance lead times of orders in a supply chain simulation. This means that multiple runs are required to estimate the mean result according to Eq. 13. Furthermore, either the data need to be normally distributed or n needs to be sufficiently large.

Additionally, it is of importance to eliminate the commonly observed initial transient phase of simulation runs. An initial transient phase may for instance be observed in a supply chain simulation, where initial order lead times may be significantly shorter compared to the lead times of later orders, due to the fact that the system is idle in the beginning of a simulation run. There are several methods for elimination of the initial transient phase (Lavenberg et al. 1981).

Thorough analysis of output data is essential when experimenting with simulation models. For detailed information about this topic, including for instance methods for hypothesis testing when multiple system configurations need to be compared, see Law (2007).

– *Section IV:*

Finally, experimentation results are documented and reported and findings are utilized for decision making in the real system. Besides the rather obvious documentation of results, thorough documentation of the model itself is highly advisable, due to the probability that it may be modified and reused for future evaluations, potentially by different analysts.

4.3 Adaption of DES to chemical processes

4.3.1 Review of DES application in the chemical industry

Manufacturing industries as well as the service sector have identified Discrete Event Simulation (DES) as an effective tool for understanding and predicting process flow. DES is widely applied as decision support when designing new facilities, or optimizing operations in existing systems. A comprehensive review of the application of DES in manufacturing and business is provided by Jahangirian et al. (2010). In a more specific survey by Smith (2003), a wide range of examples of the application of DES for design and operation of manufacturing environments can be found. Despite citing numerous publications on the application of DES, both review papers only marginally mention the chemical industry. This lack of coverage, which is present in academic literature as well as corporate application, is mainly due to the fact that continuous process flow of chemical plants does not fit well with the capabilities of DES (Bangsow 2012).

However, on closer inspection, one recognizes that chemical processes exhibit many discrete operations, such as raw material supply, equipment maintenance, product packaging or quality control, which are all potentially decisive for production throughput. The potential of DES for modelling and understanding these discrete operations for process optimization has been pointed out (Cope 2010). Successful application of DES for modelling discrete operations in chemical plants has to some extent also been reported. Examples are simulation of machine failures (Sharda and Bury 2008), analytical laboratories (McGarvey, Dargatz and Dzirbik 2011), or final product tank farms (Sharda and Vazquez 2009). Simulation of entire production plants in the chemical industry mainly concentrates on batch processes, as they can be conveniently represented by DES models. DES has been gainfully applied for design and operation of batch plants (Faccenda and Tenga 1992; Watson 1997).

The ability of DES to adequately incorporate variability into process models makes it a prospective tool for comprehending important details of chemical plants with continuous flow areas as well. Even though these plants are commonly represented as a system of continuously operated process steps, their real life behaviour is commonly highly unsteady. Boundary conditions, such as raw material availability and quality, equipment failure or even variations in ambient temperature frequently effect rate changes of process flow. When analysing the effective capability of a chemical plant, understanding these rate changes may be crucial.

4.3.2 Introduction to DRS

Recent advancements of simulation software, such as Discrete Rate Simulation (DRS) in the software package ExtendSim®, provide a promising framework for transferring the strengths of DES to processes of bulk material flow.

DRS combines attributes of continuous and discrete event simulation. The state variables depend on rates of flow in the modelled system as in continuous simulation. However, unlike in continuous simulation, the state variables are not recalculated at equal time intervals, but with the occurrence of discrete events, which in practice could be a storage tank reaching its maximum filling level or the blocking of a rate in a flow process due to equipment failure.

As most contemporary DES packages, ExtendSim® DRS provides the user with a graphical interface of connectable building blocks. Essentially these rate library blocks can be categorized in flow storage, flow control and flow routing blocks. See Figure 20 for a simple demonstration model.

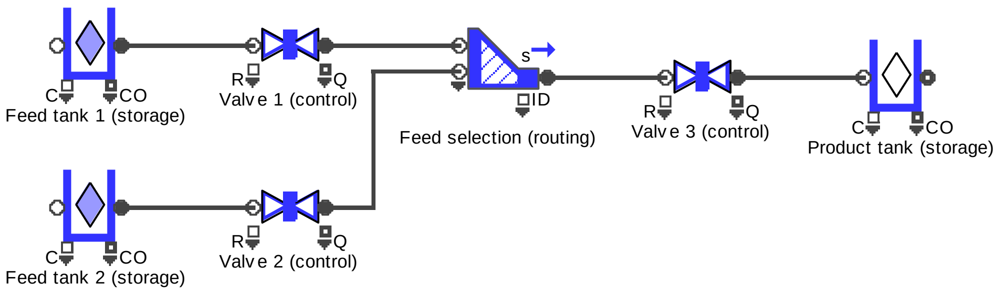

Figure 20: A simple ExtendSim® DRS model.[2]

Internally, the model is divided into rate sections consisting of connections between blocks sharing the same effective rate. These rates represent decision variables of a linear programming problem, which a Simplex algorithm seeks to maximize. The settings of the building blocks make up the constraints of the linear program. With the occurrence of each event, the linear program is revaluated and recalculated. For detailed information on the functionality of DRS, see the publication by Damiron and Nastasi (2008).

DRS holds several advantages over continuous simulation for modelling complex unsteady flow systems, rooted in its close connection to DES. As the state variables are recalculated exactly at critical events, when for example the maximum filling level of a storage tank is reached, the simulation results in the exact solution. A continuous simulation model may override the critical event in case it does not coincide with a time step and, thus, may not yield the exact solution. Furthermore, DRS minimizes the number of recalculations with its determination of critical events and in that way reduces simulation time. As DRS in ExtendSim® is integrated in a contemporary DES environment, it also contains the well-established tools of DES packages for input distribution modelling and output analysis. The modelling capabilities of DRS have been pointed out by Krahl (2009). Proof of its practical applicability is for instance provided by Sharda and Bury (2010), who used DRS modelling as part of a DES study on a chemical production process.

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4.3.3 Integration of DRS with DES and continuous modelling

As stated above, an entire chemical process hardly ever consists exclusively of continuously operated steps. For accurately modelling a complex chemical production system, one inevitably has to include sections of bulk flow as well as discrete processes. As models of DES and DRS evolve with the occurrence of discrete events, combination of both simulation concepts in a single model is straightforwardly possible, without aggravating its execution. ExtendSim® provides exchange blocks with which discrete event entities can be converted to bulk flow and vice versa. This gives the chance to easily model e.g. unloading processes at the arrival of tankers or batching of bulk material into containers.

In addition to coupling DRS with DES, integration of continuous modelling (i.e. continuous recalculation of the model at small equidistant increments of time) may also be required. In a DRS model, effective rates remain constant between two consecutive discrete events. However, in many chemical engineering applications, this does not appropriately picture the process. The flow rate or separation ratio of a particular process section (see Figure 21) may depend on continuously changing attributes and therefore vary continuously itself. For adequate representation in a DES or DRS model, discrete simulation can be coupled with continuous simulation. Several options depending on the specific case were identified and developed while elaborating this thesis. In the following paragraphs, these options according to the decision tree depicted in Figure 22 are introduced.

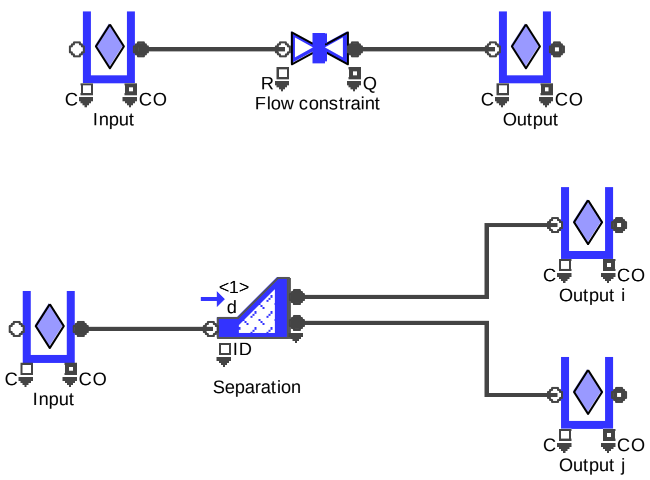


Figure 21: Operations in a DRS model which may require continuous simulation.

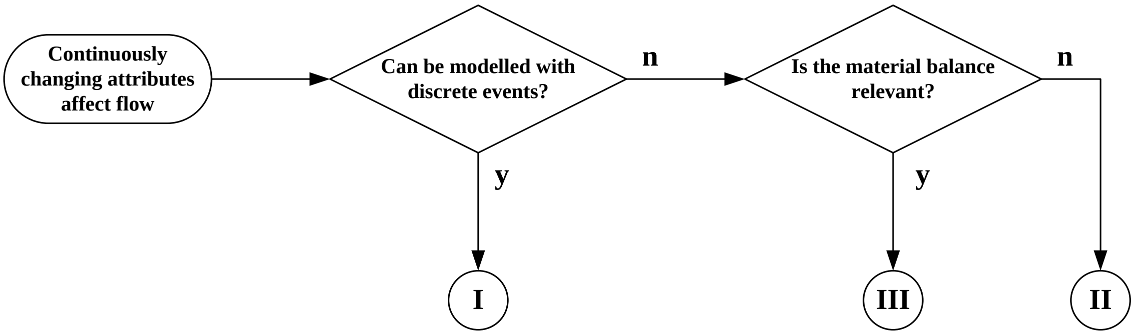


Figure 22: Decision tree for integrating continuous modelling with discrete simulation.

– *I) Modelling continuously changing flow with discrete events:*

The first question to ask is whether the continuously changing attribute, which influences the flow, can be modelled with discrete events. Adding continuous simulation to a discrete simulation model drastically increases the number of recalculations and, thus, execution time. Furthermore, it adds complexity and hereby elevates error risk. Therefore, if continuous modelling is not inevitable, its avoidance should be aspired. For instance, the effect of continuously changing ambient temperature on a separation unit could be updated only concurrently with the arrival of a new production batch. This procedure, however, must be carefully validated. For this purpose, sub-models can be built including continuous simulation and compared to the respective sub-models without continuous simulation.

– *II) Modelling continuously changing flow without material balance:*

If a continuously changing attribute needs to be integrated into the model with continuous simulation, the next question to ask is whether the attribute is dependent on the composition of the flow media. If this is not the case, subsections of continuous modelling can be introduced, in which the continuously changing attribute is directly addressed. Option II may be suitable whenever the root cause for continuously changing attribute is not inherent in the flow media itself, like for instance the variation of pressure or temperature, or if it is merely dependent on accumulated volume of flow media. In addition to continuous recalculation points, it may also be beneficial to include discrete recalculation points in order to maintain the accuracy of the discrete simulation model (cf. Krahl 2009). An example for modelling continuously changing flow without material balance in a discrete simulation model can be found in case study 3 presented in Section 5.3.

– *III) Modelling continuously changing flow with material balance:*

  If the continuously changing attribute depends on the composition of the flow media, the material balance needs to be traced through the model. In that case, not only the subsection containing the continuously changing attribute, but all the subsections upstream of the continuously changing attribute may have to be recalculated continuously. The root cause for composition variation may for instance be another continuously changing attribute such as pressure or temperature in a process step further upstream. It may also be a type of parameter variation at discrete points in time, such as batches of raw material with varying composition. In case interconnected tanks, these discrete parameter changes effect continuous changes through backmixing further downstream in the process. Modelling continuously changing flow with material balance is applied in case study 4 presented in Section 5.4.

4.4 Review of the application of DES for enhancing VSM

The profit of incorporation of DES into VSM projects has already been pointed out by various authors. For instance, Grimard, Marvel and Standridge (2005) state that simulation is able to reduce the time required between redesign and full production capability. Lian and Van Landeghem (2002) see benefits of DES for both, cost-saving and worker training prior to future state implementation. Later on, they developed a model generator, which automatically transforms static current and future state maps into dynamic simulation models (2007). Solding and Gullander (2009) present a similar approach, in which they generate a simulation model from spread sheet based VSM. Several authors apply DES to quantify the effect of VSM implementation on Lean performance measures, such as work in process and lead time (Abdulmalek and Rajgopal 2006, Detty and Yingling 2000, McDonald, van Aken and Rentes 2002).

Marvel and Standridge (2009) even postulate, that iterative Lean implementation as propagated by many authors, is inherently oppositional to Lean concepts because it is a wasteful process. Consequently they suggest future state validation through simulation in order to eliminate this wasteful process.

One issue which has not yet been addressed is the fact that VSM implementation affects conflicting cost components. However, as discussed in Section 3.4, taking them into account is crucial to measure the benefit of VSM projects, especially with chemical processes.

4.5 Development of a DES enhanced VSM procedure for complex production environments

In order to maintain the undoubtable strengths of the method, surrounding its visual and straightforward character, it is highly favourable not to overcomplicate the mapping procedure itself. Application of sophisticated simulation tools while capturing the current state and developing potential future states may jeopardise the involvement of important process experts. Thus, an enhanced method is proposed, which applies DES after the future state map is completed. The changed procedure seeks to compensate the two major deficits of classical VSM through simulation analysis:

- *Feasibility analysis* – is the proposed future state able to meet the customer demand?
- *Trade-off analysis* – does the proposed future state result in the optimal process when all cost components are considered?

The advanced VSM procedure (see Figure 23) may help to avoid iterative implementation likely to result in customer dissatisfaction and to find the global cost optimum. While most previous research has focused on checking feasibility and showing the effect of potential future state maps on typical Lean measures, the newly developed approach emphasizes on the importance of including all important cost components in a trade-off analysis. This is particularly important, because it facilitates determination of the actual quantitative benefit, which is often essential for gaining management acceptance.

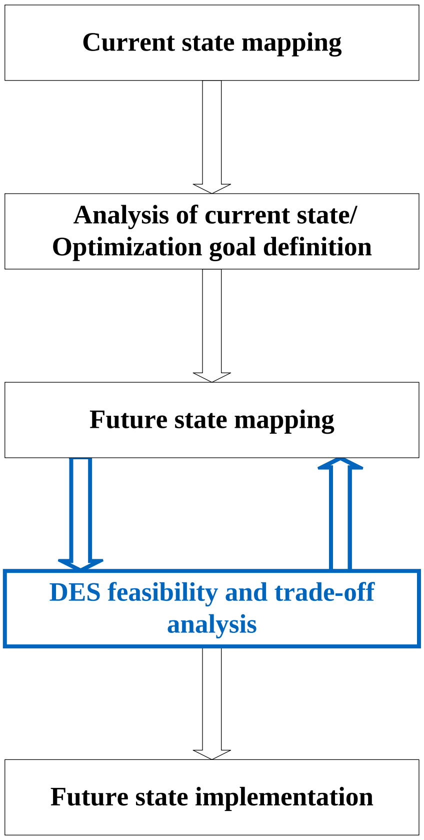


Figure 23: DES feasibility and trade-off analysis enhanced VSM procedure.

For carrying out DES feasibility and trade-off analysis, the advanced VSM procedure involves the following steps after the future state mapping phase:

- Identify variability of process data summarized in VSM and fit statistical distributions wherever possible.
- Identify cost components which are affected by future state implementation, such as tied capital, cost of poor quality, raw material and energy costs, labour costs, etc.
- Establish relationship between cost components and process measures, e.g. tied capital and inventory or energy costs and machine runtime.
- Implement the current and future state map including process data variation in a DES model, preferably with the use of contemporary DES packages.
- Verify and validate the simulation model (see Law 2007). Validation should be performed by thorough comparison of current state model with actual current state process.

– Conduct simulation experiments with the future state model and record customer order fulfilment and service level (feasibility analysis) and production costs from cost components and process measures (trade-off analysis).

The full procedure of the DES feasibility and trade-off analysis enhanced VSM method follows the steps of a common DES study, as explained in Section 4.2. Distribution of all steps over the four sections as introduced in Figure 17 is presented in Figure 24. Current state and future state mapping can be regarded as model conceptualization, as they serve as direct input for the DES model. They also serve as data collection, along with additional variability and cost component analysis. Afterwards, the simulation model is then implemented, verified and validated based on the mapping results. Experimentation with the simulation model then focuses on feasibility and trade-off analysis. The only deviation from common DES studies is a potential loop from simulation results (section III) back to future state mapping (section I). In case the simulation results are dissatisfactory, they can serve as a basis for redevelopment of the future state map. Otherwise, the proven feasibility and quantified benefits can be used to gain management acceptance before the future state of the real process is implemented.

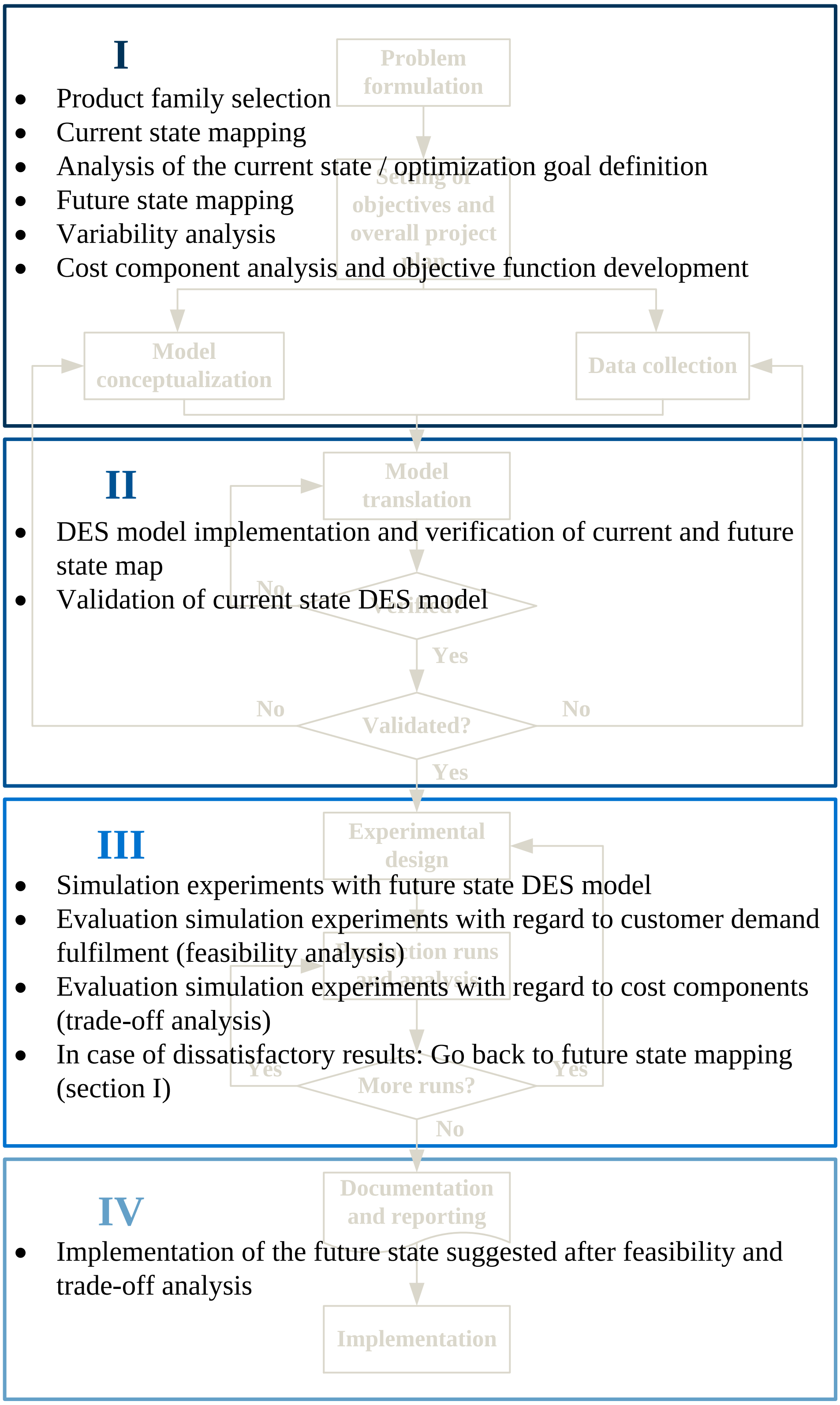


Figure 24: Steps in a DES feasibility and trade-off analysis enhanced VSM study (cf. Banks et al. 2009).

5 Case studies

In the following sections, four case studies are presented, in which Value Stream Mapping and Discrete Event Simulation is applied for optimization of chemical production processes. The case studies, which tackle specific optimization problems, serve to prove applicability of the above introduced concepts in the chemical industry.

Case study 1 in Section 5.1 provides details about a VSM project conducted for a catalytic converter production process. Here, the classical VSM approach as introduced by Rother and Shook (1999) is applied. The process contains elements of both discrete part manufacturing as well as chemical production. The purpose of this case study is to demonstrate the applicability of VSM in the chemical industry. On the one hand, the case study illustrates the benefit of VSM. However, on the other hand, it also reveals several deficits, which led to the development of the DES enhanced VSM procedure introduced in Section 4.5.

Case study 2 in Section 5.2 gives insights into a DES enhanced VSM project conducted for a high volume catalytic converter production process. Both, the feasibility and trade-off analysis as elaborated in Section 4.5 were applied during the project. The purpose of the case study is to prove the applicability and to demonstrate the benefit of the DES enhanced VSM method.

Case study 3 in Section 5.3 focuses on demonstration of DES as a valuable tool for decision support in holistic optimization of chemical processes. For this purpose, an exemplary three stage chemical production process is implemented in an integrated DES, DRS and continuous simulation model. Based on multiple cost components, an objective function is elaborated. For solving the objective function, an Evolutionary Strategies algorithm is applied.

Case study 4 in Section 5.4 covers the deployment of DES, DRS and continuous simulation for debottlenecking of a complex chemical waste water treatment and byproduct isolation process. The process stretches out over three different, individually operated plants, containing both batch and continuous processing steps. The purpose of the simulation model is to find feasible solutions for capacity increase of the process. It serves as an example for how the simulation techniques can be utilized for understanding process flow in complex transient environments.

With the exception of case study 3, this section gives insight into projects conducted within the Clariant Business Unit Catalysts. For confidentiality reasons the data presented in the following subsections are partly made anonymous through modification or negligence of figures.

5.1 Case study 1: Application of VSM in a catalytic converter production process

Catalytic converters transform toxic components of exhaust gas into less toxic compounds by catalysing redox reactions. Depending on the specific application, these reactions include for instance oxidation of CO to CO_2, oxidation of unburned or partially burned hydrocarbons to CO_2, or reduction of nitrogen oxides to N_2. Generally speaking, catalytic converters consist of three different components (see Figure 25), a monolithic substrate, the washcoat and the catalytically active species. The monolithic substrate, which has a honeycomb structure, provides the support system for the catalyst. It commonly consists of either cordierite ceramic or metal foil. The washcoat consists of oxides such as alumina or titania with fine particle size. It is coated on the channels of the monolithic substrate and, with its high surface area, maximizes the surface available for chemical reaction. The catalytically active material is applied to the washcoat oxides. It commonly consists of one or more metal species, for instance Platinum Group Metals (PGM) such as Platinum, Palladium and Rhodium, or Vanadium.

The production process of catalytic converters in this case study consists of preparation of the washcoat including the catalytically active component, and its application to monolithic substrate. It is described in detail below.

The VSM project elaborated in this case study covers the selection of the product family, composition of the current state map and development of the future state map. It is followed by a discussion on the benefits as well as deficits of VSM, specifically for the process in focus.

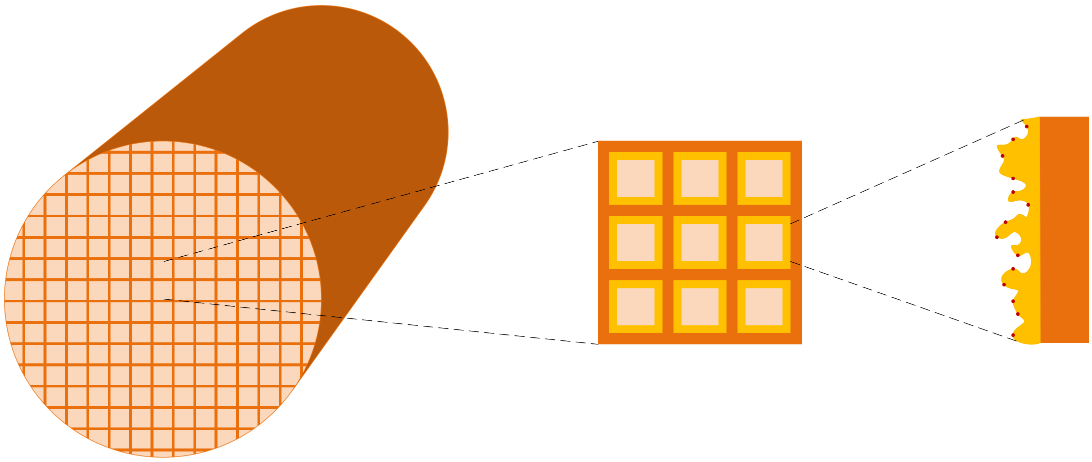


Figure 25: Structure of catalytic converters, including monolithic structure, washcoat and catalytically active species.

5.1.1 Selection of a product family

At the catalyst production site in focus of case study 1, catalytic converters are produced in two different plants (plant A and plant B). The catalytic converter production includes catalysts for automotive off-gas purification (mainly produced in plant A) as well as catalysts for industrial off-gas purification (mainly produced in plant B). For setting the scope of the VSM project, first a product family matrix was composed. Table 6 shows this product family matrix, which includes all major products and available process steps. Analysis of the matrix resulted in the definition of five product families. For confidentiality reasons, these product families are here labelled product family A, B, C, D and E.

For the VSM project of this case study, product family A was selected. It consists of three major products, which are available in several variants. The products are related to each other in several ways. As can be seen in the product family matrix, they have multiple process steps in common. Furthermore, they are also mainly produced in plant A with the same or similar equipment. The catalytic converters of product family A also serve the same application, the removal on of nitrous oxides automotive heavy duty diesel engines by selective catalytic reduction (SCR).

Table 6: Product family matrix of catalytic converters in case study 1.[3]

Product	Thermal pretreatment 1	Thermal pretreatment 2	Thermal pretreatment 3	Primer coating	Primer calcination	Powder impregnation 1	Powder impregnation 2	Powder calcination 1	Powder calcination 2	Ball milling 1	Ball milling 2	Toothed colloid milling	Dip coating 1	Dip coating 2	Dip coating 3	Pump coating	Honeycomb calcination 1	Honeycomb calcination 2	Spray impregnation 1	Spray impregnation 2	Dip impregnation 1	Dip impregnation 2	Honeycomb calcination 3	Dip impregnation 3	Dip impregnation 4	Honeycomb calcination 4	**Product family**
1			x									x			x			x									**A**
2			x												x			x									
3			x				x		x	x					x			x				x	x				
4										x			x				x				x		x				**B**
5										x			x				x				x		x	x		x	
6											x		x				x		x	x			x				
7											x		x				x				x		x				
8										x			x				x				x		x				
9										x			x				x				x		x				
10	x									x				x			x					x	x				**C**
11	x									x				x			x					x	x		x	x	
12	x									x				x			x					x	x				
13	x									x				x			x					x	x		x	x	
14		x		x	x						x			x			x		x	x			x				
15											x			x			x		x				x				**D**
16						x		x			x					x	x										**E**

5.1.2 Current state map

Product family A consists of the three products, which for confidentiality reasons are labelled product 1, 2 and 3. For these products, variants differing in geometry or honeycomb structure are available. The products are shipped to different system integrators, who are responsible for canning of the coated honeycombs, before they are incorporated into the exhaust tract of diesel engines at a single end customer. The final exhaust gas SCR system consists of three product 1, two product 2 and one product 3 catalytic converters. An overview of the number of variants as well as the annual customer demand is presented in Table 7.

Product 1 and product 3 are shipped to the same system integrator. These products are ordered lot-wise, always in multiples of 24 catalytic converters. The system integrator provides a half year forecast which is updated weekly. Product 2 can be shipped to two different system integrators, which submit orders quarterly.

[3] Please note that only core process steps are included in Table 6.

The customer demand for product family A is rather unstable with high variability over time. The plant is not fully utilized and operators can be scheduled according to the given ordering situation in up to three shifts per day of eight hours each. The customer demand is summarized in Figure 26.

Table 7: Demand overview for product family A of case study 1.

Product	Number of variants	Demand/year	Number of variants
1	4	4,670	4
2	4	3,454	4
3	2	2,670	2

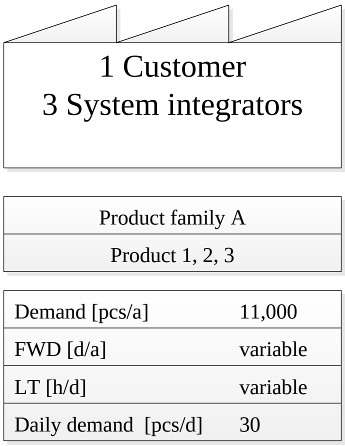


Figure 26: Customer demand of product family A in case study 1.

5.1.2.1 Process Description

The product family A products are produced lot-wise, commonly following a make-to-order rule. However during periods of elevated forecasted demand, the production rule is switched to make-to-forecast. Production takes place in plant A, with the exception of product 3, where the two most downstream process steps (PGM impregnation and PGM calcination) are carried out in plant B. The intermediates of the three products are transferred in batches from process step to process step. Batch sizes vary and are subject to daily shop floor internal scheduling.

Depending on the specific product, the following sequence of process steps is required:

(0) Thermal pretreatment (product 1, 2 and 3)

As substrates for the catalytic converters of product family A, metal foil honeycombs are used. Each product variant displayed in Table 7 requires an individual substrate. Prior to application of washcoat, the substrates are thermally pretreated. This process step, which is carried out by an external contractor, leads to roughening of surface of the foil and therefore to improved washcoat adhesion. Further information regarding thermal pretreatment as well as all further process steps is provided in the current state map of product family A in Figure 27. For confidentiality reasons, concrete data are omitted from the figure.

(1) Powder impregnation (product 3)

In order to prepare the washcoat, which is coated on the honeycomb substrates further downstream in the process, raw metal oxide powder is impregnated with an aqueous metal salt solution. The process step takes place in a planetary mixer with a capacity of 14 kg powder. One batch consists of 10 mixer runs, resulting in a batch size of 140 kg.

(2) Powder calcination (product 3)

The impregnated powder for product 3 is then dried and calcined in a batch oven. The batch size during powder calcination is 140 kg, just as during impregnation. With this amount, the oven capacity is fully utilized. The process time for one oven run amounts to 12 h. Powder impregnation and calcination are directly linked. Whenever a batch of powder is impregnated, calcination is started. Therefore no intermediate inventory is found between the two steps.

(3) Washcoat production (product 1, 2 and 3)

The washcoat for the three products is prepared by mixing oxide powders with deionized water, yielding an aqueous slurry. Furthermore, organic or inorganic binders are added for enhancement of the adhesion between washcoat and metallic honeycomb. For product 1 and product 2, the catalytically active material is already contained in the oxide powder mixture of the washcoat. The washcoat for product 3 on the other hand contains oxide particles for providing surface area and stabilisation of the catalyst, while the catalytically active material is applied further downstream in the process.

After production of the slurry, the washcoat of product 1 is processed through a toothed colloid mill in order to destroy agglomerates. The washcoat of product 3 is milled with a ball mill in order to adjust primary oxide particles to the desired particle size distribution. Finally, the washcoats are stored in drums on the shop floor. Process measures of washcoat production can be found in in Figure 27.

(4) Substrate labelling (product 1, 2 and 3)

Before coating, the thermally pretreated metallic honeycombs are unpacked and labelled. They are then set up on pallets in the batch sizes required for coating. Substrate labelling is not depicted in Figure 27.

(5) Washcoat dip (product 1, 2 and 3)

The metallic substrates are then coated with the oxide slurry in a dip coating process. The substrates are dipped into the washcoat before excess washcoat is removed from the honeycomb channels by pneumatic air-knifing. The process- and cycle time of this process step depend on the product.

(6) Honeycomb calcination – washcoat (product 1, 2 and 3)

After washcoating, the honeycomb substrates are transferred to a continuously operated belt oven, where they are dried and calcined. The belt speed, as well as the temperature profile depends on the specific product. Thus, the individual products cannot be calcined in mixed batches. For changeover, belt emptying and temperature program change are required. The process time is a linear function of the specific belt speed, while the cycle time is a function of belt speed and substrate diameter. Both figures are listed in the current state map for the individual products.

In the case of product 1 and product 2, process steps 5 and 6 are repeated in order to achieve the desired oxidic loading on the substrates.

(7) PGM impregnation (product 3)

The product 3 intermediates of honeycomb substrates coated with oxides are then transferred to plant B, where they are impregnated with a PGM solution. This process step cannot take place in plant A due to cross contamination risk restrictions. Transportation is estimated as 30 min per batch of 24 pieces.

(8) Honeycomb calcination – PGM (product 3)

The impregnated honeycomb substrates of product 3 are then calcined in a batch oven in plant B. The batch oven has a capacity of 18 or 30 pieces depending on the product variant. The process time amounts to 12 h.

(9) Conditioning (product 1)

The coated and calcined honeycombs of product 1 are freed of residual oxide particles, which do not adhere to the metal foil. For this process step, the substrates are clamped into a specially designed apparatus, in which they are lifted and dropped.

(10) Packaging (product 1, 2 and 3)

The final products are packaged in cardboard boxes and tied up in batches of 24 pieces on pallets before they are shipped. Packaging of product 1 and product 2 takes place in plant A, while product 3 is packaged in plant B.

5.1.2.2 Process flow and inventory

Production of the catalytic converters of product family A is scheduled shop floor internally by a shop floor supervisor. The raw material is ordered by the supply chain management (SCM). While raw material is ordered monthly in constant amounts based on a one year forecast, production is scheduled with a make-to-order strategy. SCM and production scheduling are continuously in contact in order to respond to irregularities in the customer demand. E.g. SCM can depart from levelled monthly ordering when the customer demand decreases, or production scheduling can be switched from make-to-order to make-to-forecast when the demand forecast peaks.

Even though plant A of the catalytic converter production at the site is designed for flow processing, including continuously operating equipment such as a belt oven, the actual process has a strong job shop character. This is mainly due to the relatively low utilization of the plant. When VSM calculations are applied to job shops environments, care must be taken (Alves, Tommelein and Ballard 2005). E.g. calculation of PLT by Little's Law as introduced in Section 3.2.2 is valid for steady state processes and may be applied for comparably static, continuous throughput. However, shop floor inventory of product family A products is highly dynamic. With some exceptions, whenever a job (= batch of a specific product) is started, it is channelled through all process steps before the consecutive job is processed on the shop floor. Instead of the integral approach provided by VSM, direct measuring was applied for determining the PLT of metal substrates on the shop floor (see Table 8). For the overall site on the other hand, PLT or DOI calculation according to Little's Law was found to be more meaningful. Due to the levelled ordering of raw material by SCM, compared to the shop floor, the overall site inventory remains rather stable over time. Raw material as well as final product inventory, DOI calculated by Little’s Law and amount of tied capital is presented in Table 9.

Table 8: Current state shop floor PLT of metal substrates for product family A of case study 1 between washcoat dip and packaging (PLT determined by process tracing).

Product #	Av. PLT [d]	Min. PLT [d]	Max. PLT [d]
1	2.7	1	5
2	1	1	1
3	17.8	10	22

Table 9: Raw material and final product inventory of product family A in case study 1 (DOI calculated by Little’s Law).

Material	Inventory	PLT [d]	Tied capital [€]
Product 1 raw substrates	633 pcs	49	225,000
Product 2 raw substrates	594 pcs	81	72,000
Product 3 raw substrates	313 pcs	33	77,000
Product 1 raw oxides	3395 kg	100	40,000
Product 2 raw oxides	496 kg	912	4,000
Product 3 raw oxides	192 kg	41	16,000
Product 1 final product	399 pcs	31	214,000
Product 2 final product	-	-	-
Product 3 final product	76 pcs	8	32,000

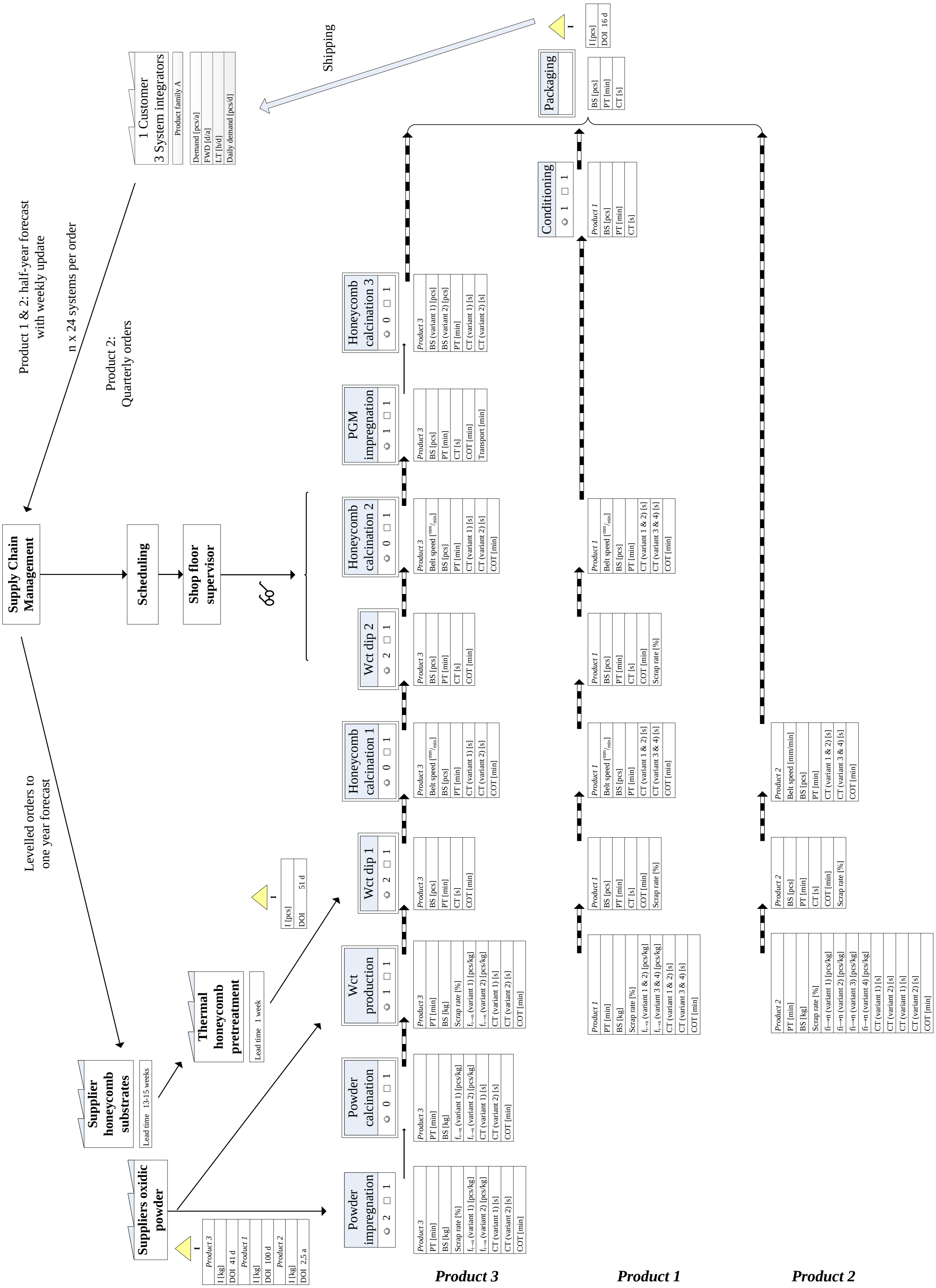


Figure 27: Current state map of product family A in case study 1 (for confidentiality reasons, concrete data are omitted).

5.1.2.3 Analysis of the current state

(1) Process Lead Time

PLT was calculated by Eq. 8. Since no shop floor inventory was found due to the transient character of the process, only raw material and final product inventory were included in the PLT calculation (summarized in Table 10). It had to be taken into consideration that inventories of product family A products are dynamically built up and worked off over time. Therefore the data only depict a snapshot of the production process. Nevertheless, the static lead time calculation gave fruitful indication of inefficiencies in the value stream.

(2) Flow Ratio

The flow ratio of product family A products is presented in Table 10. Since the process was commonly operated with only one shift per day, an adjusted calculation of the flow ratio was applied. As not 24 hours were available for flow, the denominator was diminished by the available 7.5 h labour time per 24 h (see Eq. 14). Flow ratio calculation of product family A products, as the PLT calculation gave a snapshot of a highly transient process. However, even though the figures were not valid for all catalytic converters processed, they did provide information of the available room for improvement.

$$FR = \frac{\sum_{Step\ 1}^{Step\ n} PT}{PLT \cdot \frac{labour\ time}{total\ time}} \qquad \text{Eq. 14}$$

Table 10: Process lead times and flow ratios of product family A in case study 1 (raw substrates to final product).

Product	PLT [d]	FR
1	80	1.5 %
2	81	0.2 %
3	41	5.0 %

(3) Operator Balance Chart

With the operator balance charts in case study 1, a peculiarity of chemical processes becomes apparent. Intermediate recycle as applied for product 1 and product 3 add complexity to the creation of the chart. Here, two options were found to be available. A process step based operator balance charts in which the cycle time of all individual process steps regardless of equipment gives hints about process flow between adjacent process steps. However, it does not necessarily show overall process bottlenecks. An equipment based operator balance chart on the other hand, in which cycle times of different process steps on the same equipment are summed up, indicates overall process bottlenecks, but does not directly show flow behaviour on the shop floor. The problem gets even more sophisticated, when material streams are parted and only fractions are recycled.

For product family A products, process step based operator balance charts were chosen, due to the fact that the shop floor process steps are underutilized and no equipment bottlenecks operating above the takt time were to be expected. The charts displayed in Figure 28 show significant differences in cycle time among the steps. Detailed evaluation and process improvement proposals are provided below.

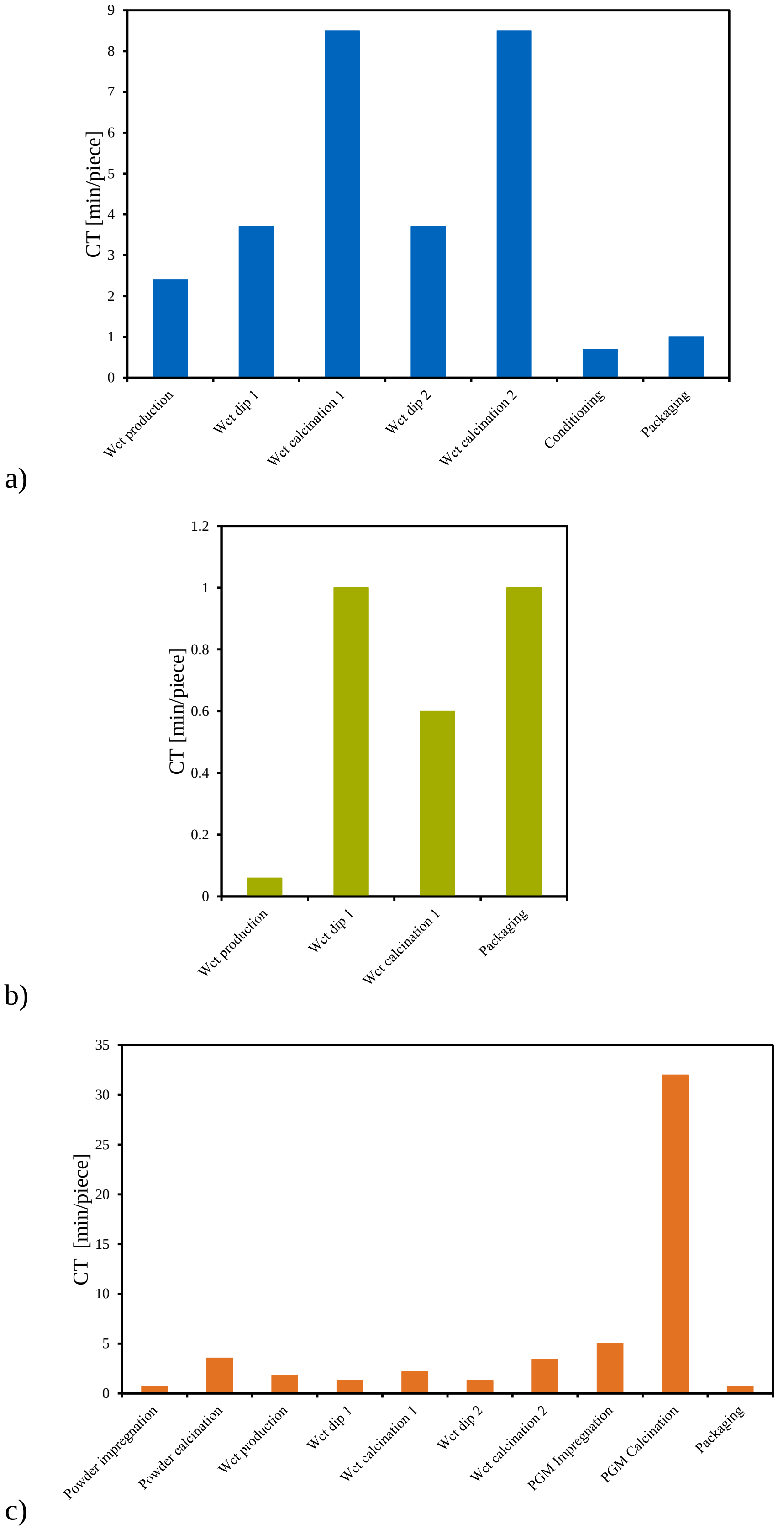


Figure 28: Operator balance charts of product family A products of case study 1. product 1 (a), product 2 (b) and product 3 (c)

5.1.3 Future state map

Top priority of the elaborated future state for product family A products was a decreased lead time and reduced inventory. The inventory of major raw materials and final products recorded in the current state map accounted for 680,000 €. Elaboration of the future state map is structured into two subsections. First proposals for the shop floor process are given, before the overall supply chain including suppliers and delivery to the system integrators is investigated.

5.1.3.1 Shop floor future state

Even though the shop floor process does not contribute significantly to the overall lead time of the process (compare Table 8 to Table 9), it does create turbulence through varying flow, impeding a reliable process through the overall supply chain. In order to improve the shop floor process, applicability of the VSM future state guidelines was evaluated.

Guideline 1, synchronization of the process with the takt time, was found to be not applicable. As the process is operated well below design capacity, product family A production is shut down and operators are assigned to different plants when no orders are due. Continuous operation of the process would have significantly lowered productivity and was therefore not considered.

Guideline 2, creating continuous flow through process integration and FIFO, was found to be applicable for several process steps:

- *Substrate labelling, weighing and washcoat dipping:*

  In the current state, the raw metallic substrates are unpacked from cardboard boxes, labelled and weighed, before they are stacked on pallets (not depicted in Figure 27). Washcoat dipping is decoupled from the labelling process step and takes place at a different point of time. When integrating both process steps, the cycle time is increased, in case no further operators are added. However since the successive process step of product 1 and product 2 (washcoat calcination) has a significantly higher cycle time than washcoat dipping (see Figure 28 a and c), the overall process is not decelerated by this measure.
- *Washcoat dipping and washcoat calcination:*

  The gap between the cycle times of washcoat dipping and washcoat calcination in the current state impedes efficient process integration of the two steps.

However, through a process optimization project, the cycle time of calcination was significantly lowered through temperature and ventilation adjustments, making process integration feasible.

– *Powder impregnation, powder calcination and washcoat production:*

  In the process of product 3, powder impregnation and powder calcination, which are already coupled in the current state, could be integrated with washcoat production. Due to the fact that the washcoat has a certain shelf life, the batch size of washcoat production is considerably lower than the batch size for impregnation and calcination. Integration of the steps therefore entails lowering of the batch size for impregnation and calcination, leading to increased specific energy consumption, a trade-off which is out of scope in case study 1.

– *Process steps downstream of washcoat calcination:*

  For several reasons, such as location distance and cycle time differences, integration of the process steps downstream of washcoat calcination was found to be impractical. Instead, introduction of FIFO with accumulation limit can be suggested in order to ensure steady processing.

Guideline 3, implementing supermarket pull systems where continuous flow is not possible, was found to be applicable between washcoat production and washcoat dipping. This process change guarantees constant supply of washcoat without inventory build-up and scheduling efforts.

Guideline 4, scheduling only at one process step, was also found to be applicable. As the pacemaker process step, the first washcoat dip is selected, because the downstream process steps operate with continuous flow and from upstream steps material is pulled.

Guideline 5, levelling the production mix, was not found to be practical. As the process downstream of the pacemaker is scheduled make-to-order under normal circumstances, even distribution of products on the schedule was not considered.

Guideline 6, releasing and withdrawing small and consistent increments of work at the pacemaker, was again found to be applicable. An initial pull system is proposed for the process steps between the first washcoat dip and the final washcoat calcination (product 2 and 3) or conditioning (product 1). Only when one shop floor order is completed at the final step, another order is released at the pacemaker. The shop floor order increments of work are dimensioned to occupy the process for one shift.

Guideline 7, producing every product within the smallest possible intervals of time, was not considered. Due to the fact that changeovers at the calcination step entail complete emptying and temperature profile adjustment of the belt oven, they are both time and energy consuming. Therefore reducing the release order increments below the workload of one shift was found to be impractical.

The shop floor improvement measures are summarized in a qualitative future state map, displayed in Figure 29. Compared to the current state of the shop floor process, the future state yields reduced scheduling efforts. Furthermore, low, reliable lead times are achieved (compare Table 11 to Table 8). Theoretically, when no breakdowns occur, PLT from the first washcoat dip to packaging does not vary due to the initial pull system with consistent increments of work released to the shop floor.

Table 11: Future state shop floor PLT of metal substrates for product family A in case study 1 between washcoat dip and packaging (PLT determined by process tracing).

Product #	PLT [d]
1	1
2	1
3	3

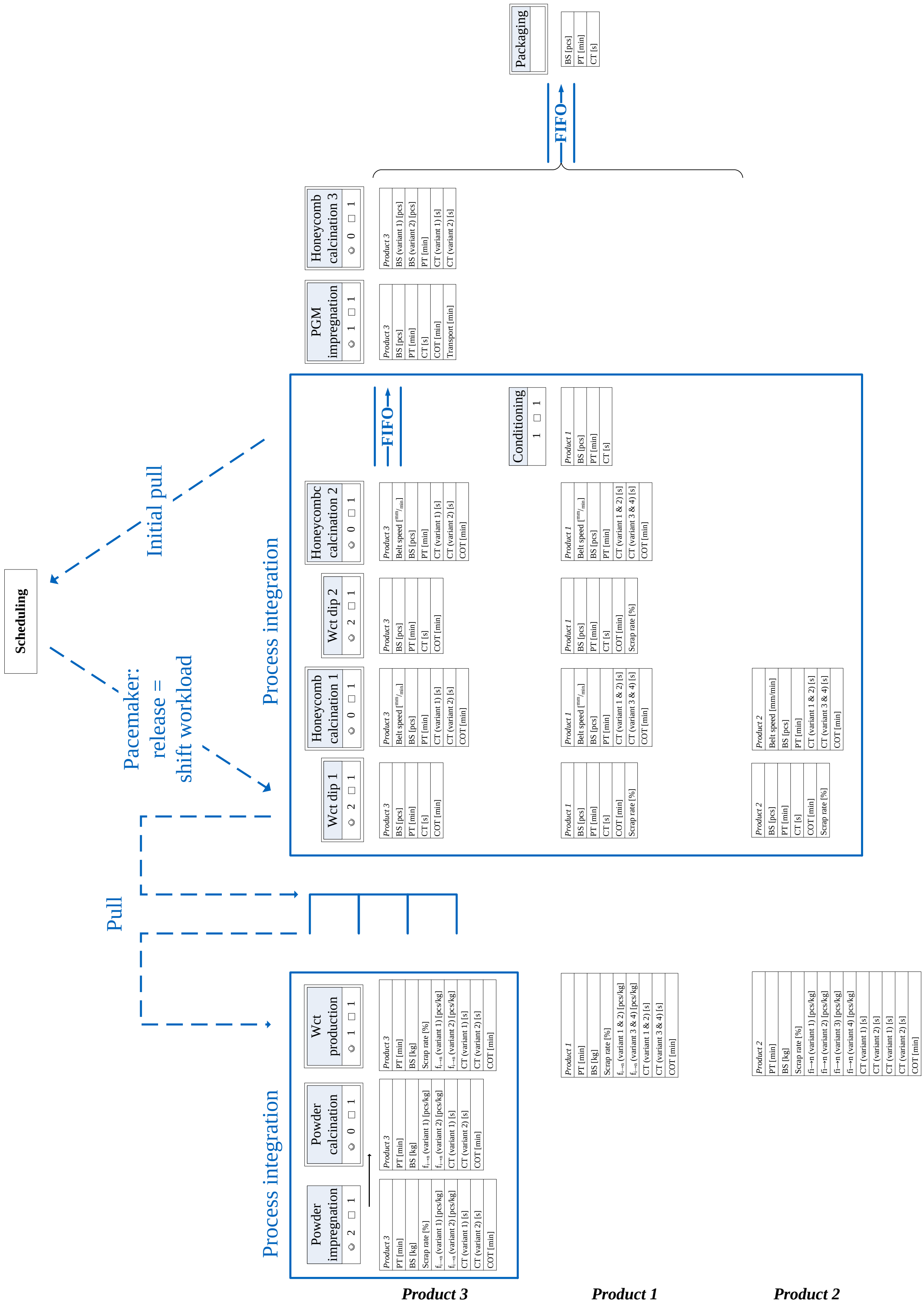


Figure 29: VSM future state map for the shop floor process of product family A in case study 1 (for confidentiality reasons, concrete data are omitted).

5.1.3.2 Supply chain future state

The major drawback of the current situation of the supply chain process was found to be the gap between the overall lead time and the delivery dates demanded by the customer. When producing with a make-to-order strategy, fulfilment of the following constraint is crucial:

$$PLT\Big|_{supplier}^{customer} \overset{!}{<} due\ date - order\ date \qquad \text{Eq. 15}$$

Strict make-to-order production is only possible, if the overall process lead time including all steps in the process from raw material ordering to inventory residence times and shop floor process steps is shorter than the response time provided by the customer between incoming order and due date. A current state map of product family A catalytic converters, focusing on the overall supply chain process while simplifying plant internal processes is provided in Figure 30. Especially for product 1 and product 3 the disadvantageous situation is made clear. Already the first two external steps, raw honeycomb substrate ordering from the supplier and thermal honeycomb pretreatment sum up to a lead time of 14-16 weeks. The response time on the other hand is uncertain. The customer provides the catalytic converter producer with a half-year forecast, which is subject to weekly changes. This situation does not allow strict make-to-order. In the current state of the process, it requires decoupling of raw material management and the actual production process. While production is strictly scheduled in accordance with fixed orders, raw material is ordered monthly in batches following the forecast.

For the future state, two potential solutions are proposed to avoid this drawback:

Preferably, a true make-to-order process is established by closing of the gap between lead time and response time. For this purpose, either a frozen zone for customer orders has to be negotiated and/or the lead time of raw material from the supplier has to be shortened. The make-to-order process is supported by the shop floor future state, which, with its low, reliable lead times, enables just in time planning and scheduling.

If it is not possible to negotiate conditions with suppliers and/or customers under which Eq. 15 is fulfilled, an end-to-end make-to-order process cannot be established. In this case, a pull system for raw metallic honeycomb substrate ordering is proposed. Instead of levelled orders according to the one year forecast in the current state, in the future state, new orders are only released when the inventory level (i.e. inventory on site plus inventory in transit of honeycombs already ordered) falls below a reordering point. With this procedure material is pulled into the process rather than pushed as in the current state. In order to reduce average inventory on site as much as possible while guaranteeing continuous supply, a certain safety stock has to be defined based on demand and supply variability. The safety stock plus the average customer demand during supplier PLT defines the reordering point, below which fixed quantities of honeycombs are ordered. This so-called Q,r-model (Q stands for the fixed order quantity and r for the reordering point) for designing supply chain pull systems is elaborated in in detail by Hopp and Spearman (2008) and specifically for chemical production by King (2009).

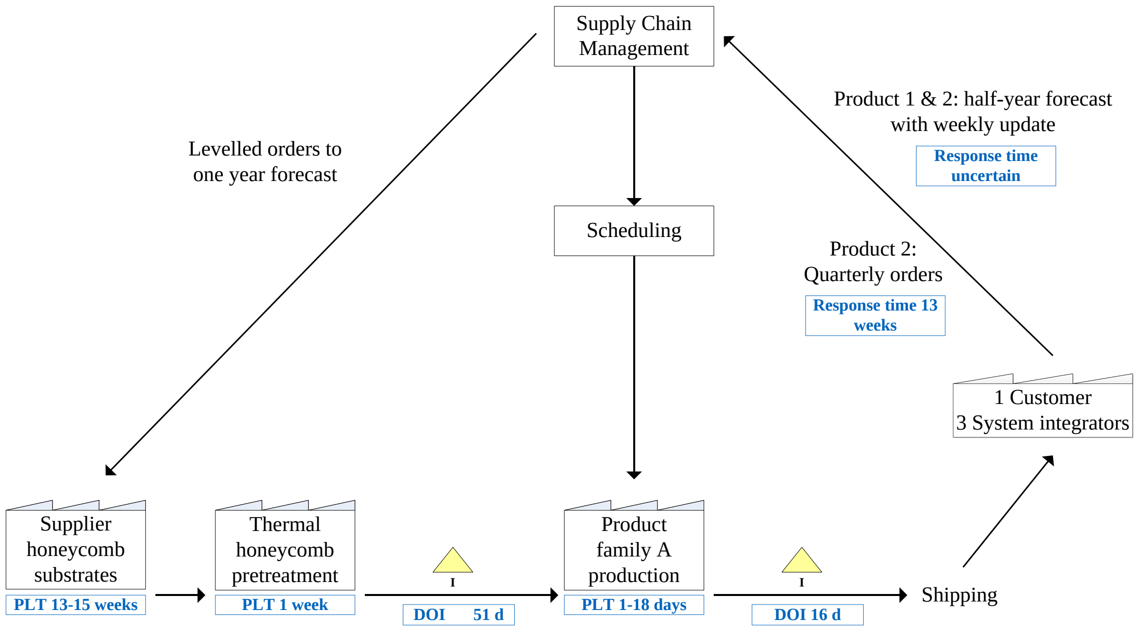


Figure 30: VSM current state map for the supply chain process of product family A in case study 1.

5.1.4 Discussion

Case study 1 covered a VSM project, which differs from its original field of application introduced by Rother and Shook (1999) in two ways. The production process in focus is operated as a make-to-order job shop. Furthermore it holds several peculiarities of chemical production.

VSM for make-to-order processes has been analysed by Alves, Tommelein and Ballard (2005). An approach for the application of VSM to make-to-order processes has been elaborated by Rother (2005). For the process of catalytic converter production of case study 1, VSM was found to be applicable for the most part. However, the low volume make-to-order process made lead time calculation by Little's law inaccurate for two reasons. On the one hand the in-process inventory level is highly fluctuating. On the other hand, the output rate of the process is variable and does not correspond to the customer demand takt time. Therefore, instead of Little's law, direct tracing of lead times is proposed in order to accurately depict the current state. Furthermore, the fact that the process is underutilized and it is scheduled according to demand led to non-application of future state guideline 1, synchronization of production with takt time, because of its negative effect on productivity.

The peculiarities of chemical production had further impact on the application of VSM. The fact that material is cycled through equipment more than once led to limitations for the informative value of the operator balance chart. As a result, the distinction between process step based and equipment based operator balance charts was discussed. As an alternative to operator balance charts, especially in chemical batch production environments, for visualization of process flow Gantt charts may be utilized. A further peculiarity of the process in case study 1 was the requirement to integrate material balances into VSM in order to accurately relate process measures to the end product. This was done with the introduction of mass correction factors as proposed in Section 3.4.2. This procedure, even though it led to increased efforts, was found to be uncritical. Finally, significant changeover efforts, including elevated energy and material consumption lead to non-application of future state guideline 7, producing every product within the smallest possible intervals of time.

Even though VSM was found to be applicable, the case study revealed the two major deficits of VSM, the lack of proving feasibility of the future state and the lack of evaluating trade-offs between conflicting cost components. The design of supermarket pull levels, FIFO lanes or initial pull increments are based on the rather static picture provided by VSM. No proof is given that the future state developed by pencil on paper is able to fulfil the customer demand. Furthermore, trade-offs between increased flexibility and reduced energy consumption were evaluated by gut feeling rather than quantitative measures. It is for instance not made clear that scheduling increments of one shift workload at the pacemaker is the most beneficial procedure. In order to overcome these deficits, the dynamics of the process need to be included in the VSM project. The DES enhanced VSM procedure as elaborated in Section 4.5 provides a promising alternative to address this prerequisite.

5.2 Case study 2: Application of DES enhanced VSM in a catalytic converter production process[4]

Case study 2 covers a production process of catalytic converters similar to the process of case study 1 elaborated in Section 5.1. The purpose of this case study is to demonstrate the gaps of classical VSM when applied to complex chemical processes and to prove the applicability as well as the benefit of the method enhanced with DES. Emphasis is in particular put on the modelling approach as well as elaboration of cost components for the trade-off analysis.

The case study process includes production of washcoat, application of the washcoat on metallic honeycomb substrates and subsequent application of catalytically active PGM species on the washcoated substrates. The catalytic converters are produced in rather high volumes in a complexly routed process. The process exhibits multiple sources of variability and involves several cost components which are potentially aggravated by VSM optimization. As explicated in Section 3.4.1, these features are not or not sufficiently addressed by the original VSM approach. The process therefore serves as a fitting example verifying the usefulness of the DES feasibility and trade-off analysis enhanced VSM method.

5.2.1 Selection of a product family

At the production site in focus of case study 2, catalytic converters are produced mainly for automotive application. The products differ from each other in type of automotive application, type and geometry of honeycomb substrate, as well as composition of washcoat and catalytically active material. Depending on the products, different production technologies are available for washcoat production, application of washcoat and catalytically active species on the substrate as well as heat treatment.

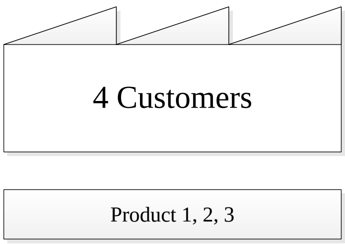
The product family selected for the case study comprises three major products with the purpose of three-way exhaust gas purification. The products share a common production technology and are produced mostly with the same equipment in the same plant. Except for a belt oven on which substrate heat treatment is carried out as well as a

[4] The content of case study 2 has been published in the International Journal of Production Research under the title „A simulation-enhanced value stream mapping approach for optimisation of complex production environments“ (Schmidtke, Heiser and Hinrichsen 2014)

honeycomb labelling machine and the quality inspection area, all equipment is dedicated to the product family in focus of the case study only.

5.2.2 Current state mapping

The three major products of the product family discussed in this case study are for confidentiality reasons are labelled product 1, 2 and 3. They only differ in geometry of the metallic honeycomb substrate as well as the composition and loading of the applied catalytically active PGM species. In addition to the three major products, there are several exceptional variants available. The products are predominantly sold to four major customers. The total annual demand for the products amounts to 804,000 catalytic converters. Even though the plant is highly utilized, significant fluctuations of the demand are observed over time. Customers provide a monthly demand forecast, which is reviewed weekly and fixed for the following week. The plant is operated on an estimated 360 factory working days and on three shifts per day with a total labour time of 21 hours per day. With the given annual customer demand of 804,000 catalytic converters per year, this results in a daily demand of 2,233 pieces, corresponding to a takt time of 33.9 s per piece. Customer demand data are summarized in Figure 31.



Demand [pcs/a]	804,000
FWD [d/a]	360
LT [h/d]	21
Daily demand [pcs/d]	2233
TT [s/pc]	33.9

Figure 31: Customer demand of catalytic converters of case study 2 process.

The production process consists of several mostly continuously operated process steps. Between the process steps, the work in process is transferred batch-wise. For the major products, the batch size is 5000 pieces (product 1) or 2500 (product 2 and 3).The process is displayed in Figure 32. It starts with the production of washcoat, consisting of metal oxides in aqueous slurry, which is mixed, homogenised and milled. Subsequently, metal foil honeycomb substrates are coated with the washcoat on two parallel machines. The coated substrates are then transferred to a continuously operated belt oven, where they are heat-treated. In order to reach the desired washcoat loading on the substrates, the coating and heat treatment process steps are repeated for two more cycles. For the third cycle, the temperature profile is changed, however the process step is carried out on the same belt oven. The substrates, coated with the final metal oxide loading are then manually placed in beakers, which are filled with a solution of the catalytically active PGM. For chemisorption of the PGM species on the metal oxide coating, the filled beakers are stored for several hours until the chemical surface reaction is completed. Afterwards, the substrates are fed to the belt oven for the fourth heat treatment step, again at a different temperature profile. The finished catalytic converters are then marked with a customer specific label on a labelling machine. Afterwards, the products are packaged in cardboard boxes. In the final shop floor step, the substrates are inspected for defects, before they are passed to the shipping department.

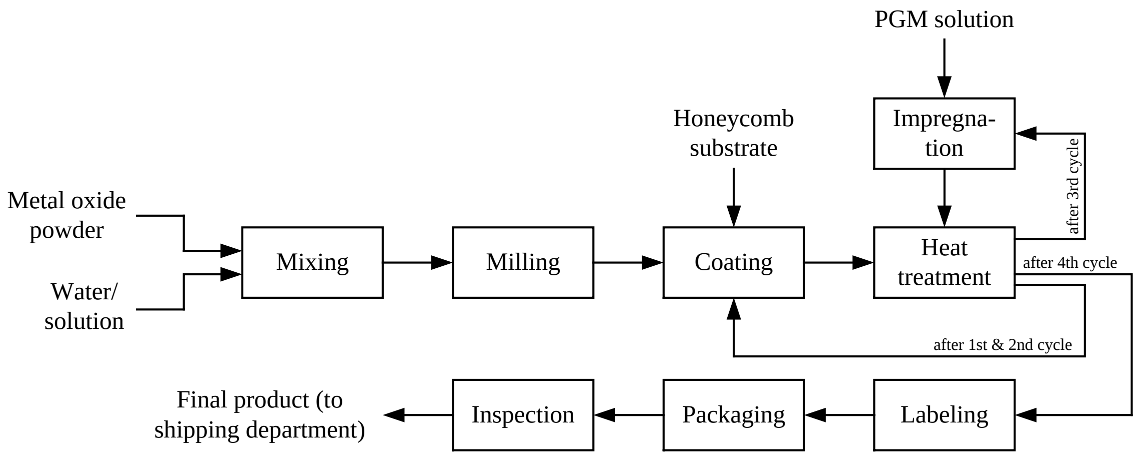


Figure 32: Process overview of case study 2 catalytic converter production.

Current state mapping data collection was conducted following the approach proposed by Rother and Shook (1999). Wherever possible, measurement of process data was carried out while walking through the shop floor. For each process step, all relevant figures, such as process time, batch time, cycle time, batch size or changeover time were collected. Between the process steps, inventory levels were counted and converted to days of inventory to provide a snapshot of current material flow.

The current state map of the product family is presented in Figure 33. The double frame of the belt oven, labelling and inspection steps indicate that this equipment is co-used by other product families, which means that its availability is limited. Note that a “go see” symbol is added to most shop floor information flow lines, meaning that the shop floor schedule on all equipment is continuously adjusted by shop floor supervisors.

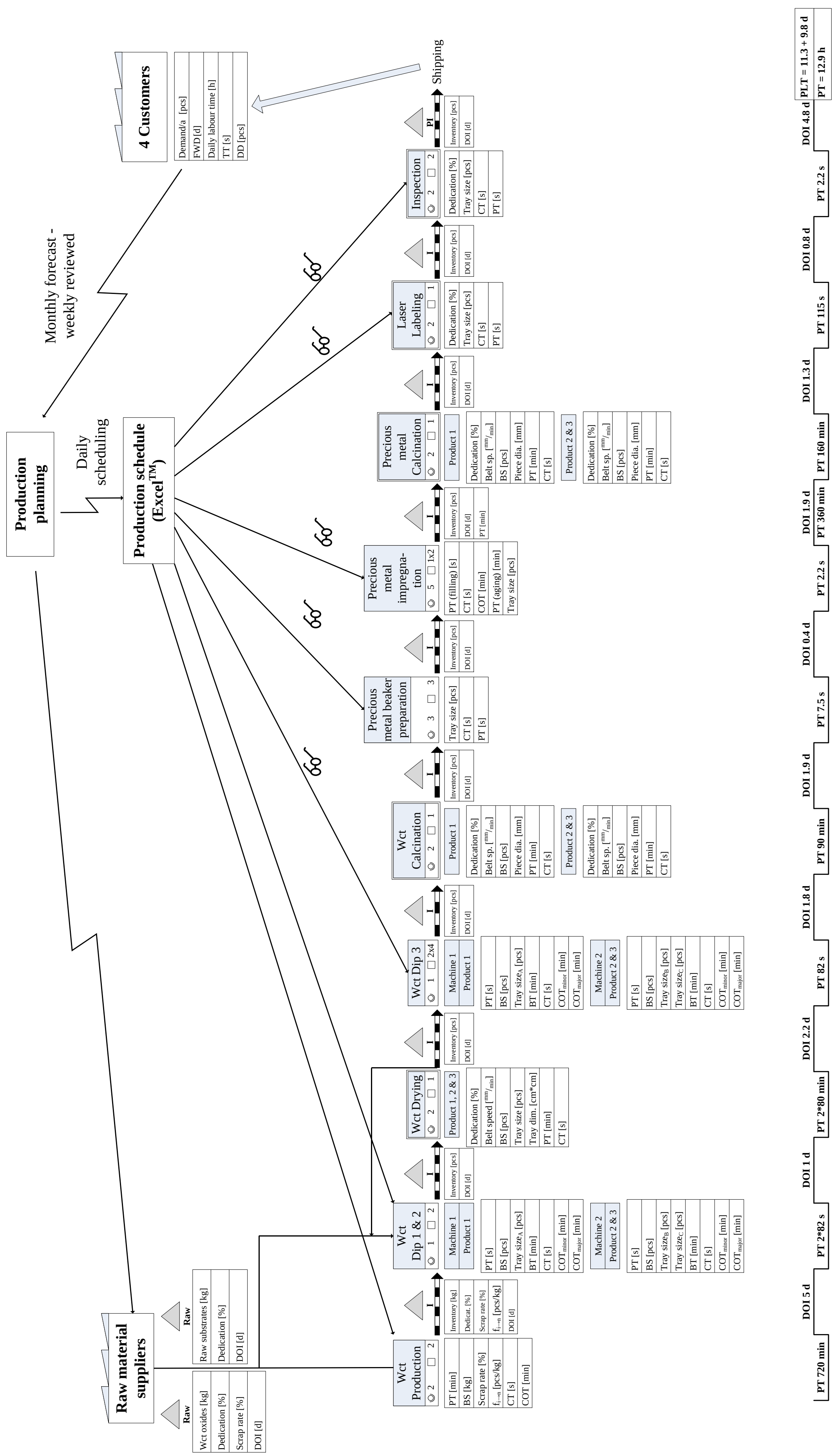


Figure 33: Current state map of case study 2 process (for confidentiality reasons, concrete data are omitted).

Due to long lead times and uncertainty of customer orders, production management reschedules daily and shop floor supervisors adjust priorities of work in process continuously. Between all individual process steps, intermediate inventory was found, adding up to 25,540 pieces for the core process from the first washcoat dip to final quality inspection. Distribution of the inventory among the process steps as found on the shop floor is provided in Table 12.

Table 12: Inventory of case study 2 catalytic converter production.

Upstream process step	Inventory level	Days of Inventory [d]
Washcoat production	70 kg oxides	5.0
Washcoat dip 1 & 2	2305 pcs	1.0
Washcoat drying	4775 pcs	2.1
Washcoat dip 3	3974 pcs	1.8
Washcoat calcination	4150 pcs	1.9
PGM beaker preparation	960 pcs	0.4
PGM impregnation	4640 pcs	2.1
PGM calcination	2930 pcs	1.3
Laser labelling	1806 pcs	0.8
Inspection/packaging	10025 pcs	4.5

Application of Little's law results in a process lead time of 11.4 days for the process between the first washcoat dip and final product inspection. The value added time as the sum of all process times for the core process amounts to 12.9 hours, yielding a flow ratio of 4.7 %. PLT and FR for various definitions of the process are summarized in Table 13.

Table 13: PLT and FR of case study 2 catalytic converter production.

Process definition (from/to)		PLT [d]	FR
First washcoat dip	Final product inspection	11.4	4.7 %
Washcoat production	Final product inspection	16.3	7.3 %
Raw honeycomb receiving	Final product shipping	30.9	2.0 %
Raw oxide receiving	Final product shipping	449.4	0.3 %

For comparing the capacity of the current state process with the customer demand, instead of the operator balance chart, a process step based capacity profile is used for case study 2 (see Figure 34). Even though lacking quantitative time information, the profile shows utilization as well as process flow in a suitable way for chemical production processes. As can be seen, the process is not constrained by overutilization, as all process steps are capable of meeting the customer demand. The highest utilization is found for the heat treatment steps as well as washcoat dipping on the second of the two available machines.

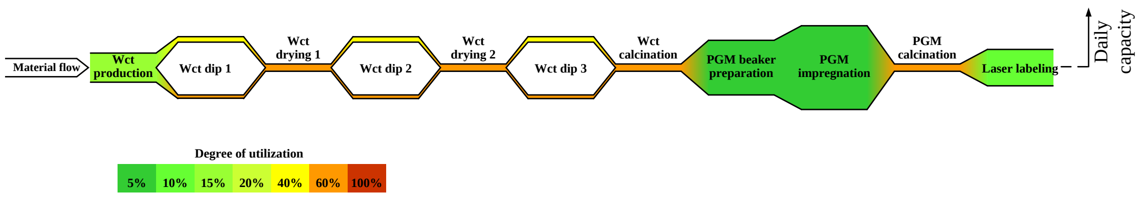


Figure 34: Capacity profile of case study 2 catalytic converter production.

5.2.3 Future state mapping

The current state map of the process reveals several shortcomings of the process, mostly related to a vicious circle around the presence of high inventory on the shop floor (see Figure 35). High inventory is directly coupled with long lead times through the shop floor process through Little’s law (Little 1961). Due to long lead times and customer demand uncertainty, continuous re-scheduling is inevitable for maintaining a high customer service level. This, in turn, results in high shop floor turbulence where flow is not governed by the FIFO rule, but by due date priority, causing high inventory. The three major downturns of this status, which can also be expressed as monetary deficits, are tied capital, high scheduling efforts and slow detection of process deterioration causing the production of defective parts.

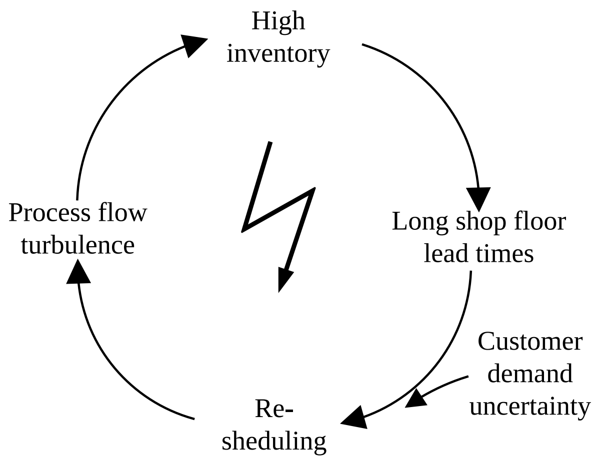


Figure 35: Relationship between shop floor issues of case study 2 catalytic converter production.

With emphasis on these concerns, the future state map was developed following the future state guidelines according to Rother and Shook (1999). First of all, the possibility of process integration was found for several process steps. ‘Precious metal beaker preparation’ and ‘precious metal impregnation’ could be directly coupled. The rather wasteful procedure of ‘packaging’ prior to ‘inspection’, which involves unpacking and re-packaging could be rearranged. This yielded the chance to integrate ‘labelling’ and ‘inspection’ prior to packaging of the final product. Between the process steps, material is piled, even though coupling of the process steps is readily possible. Process integration directly leads to elimination of the three wastes ‘transportation’, ‘inventory’ and ‘motion’ as defined by Ohno (1988).

The inventory/scheduling issue described above was tackled by batch size reduction, strict FIFO rule and introduction of initial pull. The first washcoat dip was proposed to function as the pacemaker. Upstream of the pacemaker, a Kanban pull system was suggested for washcoat production. Between the final process step and the pacemaker, an initial pull feedback control system was recommended to maintain a constant WIP level. The maximum WIP level was set to four batches. With a batch size reduction from 5,000 pieces and 2,500 respectively to 800 pieces, this results in a constant WIP level of 3,200 pieces. The rearrangements facilitate reduction of the timeframe in which a particular process step is able to process each product, which is demanded by the ‘every part every interval’ VSM future state guideline #7.

Due to the fact that the case study 2 process is non-linear, care had to be taken to keep the process effectively working, when designing the initial pull system. If the constant WIP level is set too low, the process throughput decreases below the customer takt. Based on the process data found during current state mapping as well as spreadsheet calculations, a Gantt chart analysis was used to prove that the process is capable of meeting the customer demand under steady state conditions. The analysis showed that the proposed future state is able to meet the daily customer demand of 2233 pieces. The Gantt chart for one production cycle on the shop floor is shown in Figure 36.

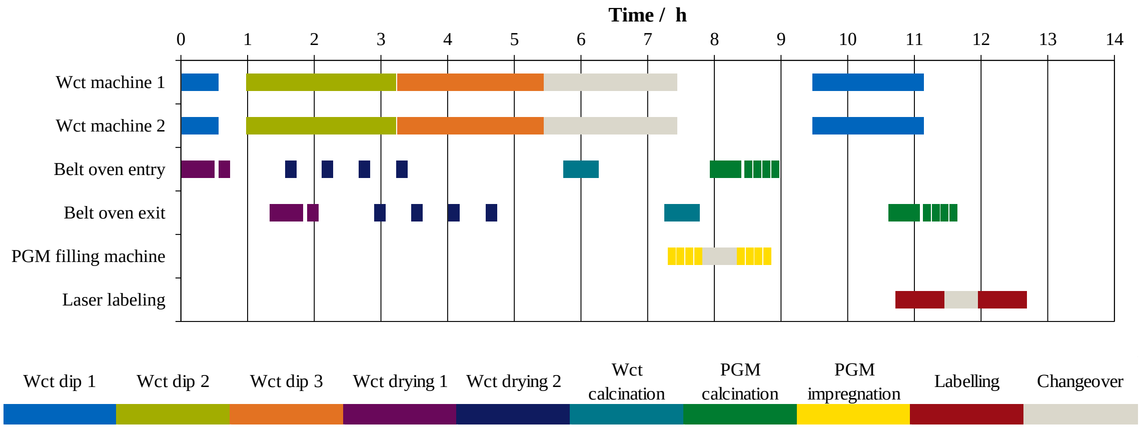


Figure 36: Gantt chart for the proposed future state of case study 2 catalytic converter production.

A simplified future state map is presented in Figure 37. All things considered, the proposed future state offers laminar production flow throughout the whole process. The WIP is drastically reduced, leading to a reduced shop floor lead time, which can be calculated as 24 hours with static spreadsheet simulation. This makes production more flexible and gives the opportunity of quick detection of errors. Furthermore, with only one process step being actively controlled, the workload of shop floor scheduling is also markedly decreased.

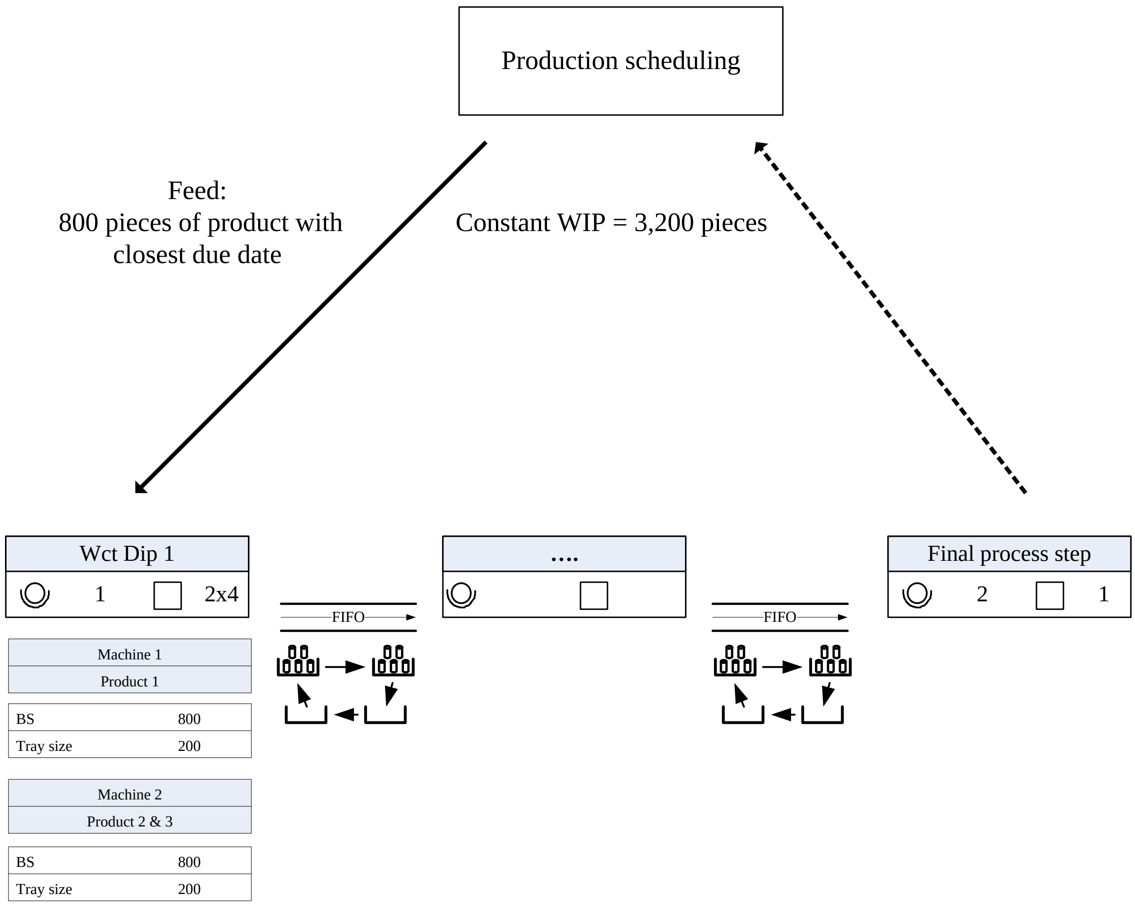


Figure 37: Simplified VSM future state map of case study 2 catalytic converter production.

5.2.4 Feasibility and trade-off analysis

After designing the VSM future state, feasibility and trade-off analysis as developed in Section 4.5 was conducted, utilizing the DES package ExtendSim®.

5.2.4.1 DES model translation, verification and validation

First, all the data determined during current state mapping were used to model the process. Additionally, variability of the process and customer demand derived from statistical analysis were modelled with appropriate distributions. After building the model, simulation of the current state was verified and validated. Verification and validation involved careful tracing of process flow, animation of the model, as well as comparison of output data with the real system. After verification and validation, the DES model enabled to adequately mimic the current state process. Observation of WIP over time for example results in a curve meandering around the level of 25,540 pieces as measured during current state mapping (see Figure 38). Simulation of the current state shows the highly transient character of the process with output data varying strongly over time.

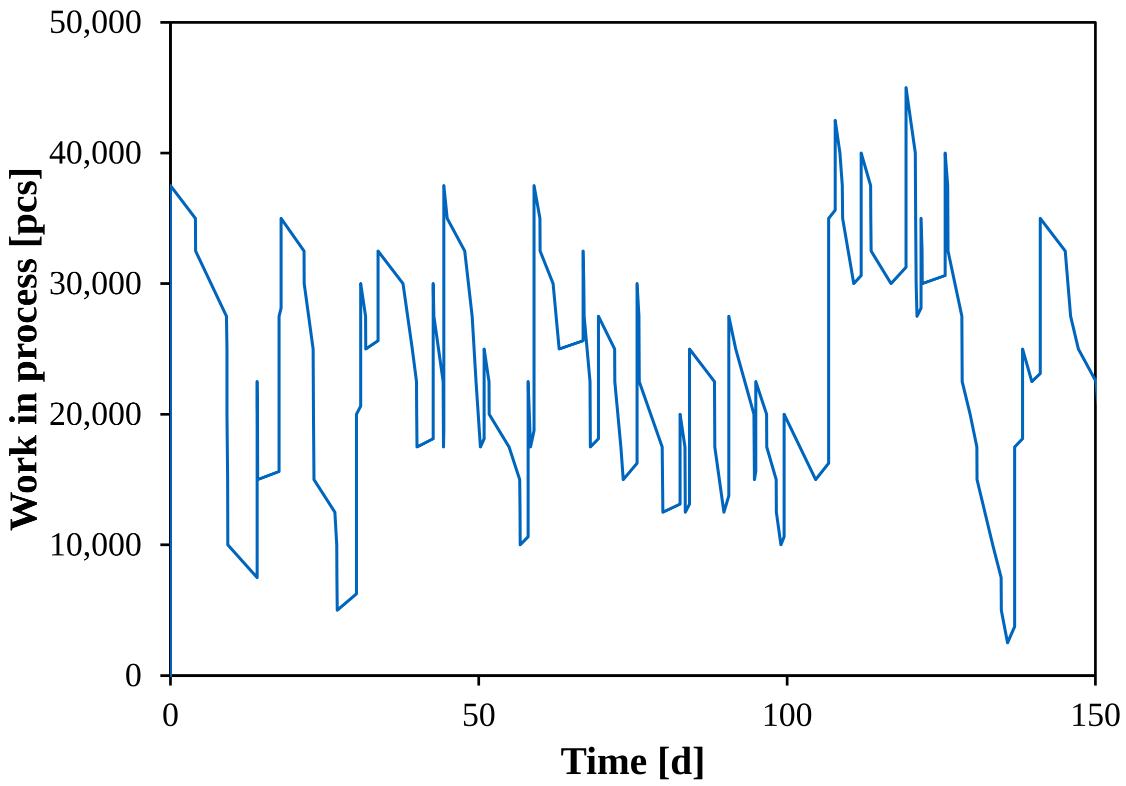


Figure 38: Shop floor WIP of the current state of case study 2 catalytic converter production.

5.2.4.2 Feasibility analysis.

In the classical VSM future state mapping phase of the case study, batch size reduction as well as initial pull with decreased WIP level were proposed. The two process modifications potentially affect the throughput, due to an increased number of changeovers and equipment idle time. The given framework of a non-linear multi-cycle process with co-use of equipment as well as customer demand variability makes the issue whether the future state is actually able to fulfil the customer demand not straightforward. Specifically, the following two questions have to be answered:

- Can the proposed future state process produce the amount of pieces demanded by the customer?
- Does the proposed future state fulfil due dates in order to maintain a sufficient customer service level as defined below?

$$Service\ level = \frac{pieces\ delivered\ on\ time}{pieces\ ordered} \quad \text{Eq. 16}$$

After validation of the current state, the model was modified in order to simulate the future state as proposed in the traditional VSM approach. Besides the proposed future state, feasibility was tested at different operating states of maximum WIP level and batch size. For comparability of the simulation results with different parameter settings, a sample size calculation was conducted. It was found that a sufficiently small 99% confidence interval for average lead time, WIP, pieces ordered, pieces processed and belt oven utilization could be achieved when the non-deterministic model was run 30 times.

The simulation results were analysed with regard to the two customer demand questions. The results show that the range of parameter settings is limited for the achievement of feasible solutions (see Figure 39 and Figure 40). The overall customer demand is not fulfilled when combinations of low batch size and low maximum WIP are applied (see Figure 39). Large numbers of changeovers and significant idle time of processing equipment make the process ineffective. The service level graph exhibits a maximum at medium WIP pull levels (see Figure 40). For low WIP levels the infeasibility can again be explained by an ineffective process causing build-up of backlog of unfulfilled orders. High WIP pull levels on the other hand result in long shop floor lead times which potentially exceed the response times given by the due date. When the process is operated at high WIP pull levels, the comparably low service level inevitably causes instability of the FIFO rule. In order to satisfy customers, rescheduling of the shop floor process is required, leading back to the problems of the current state.

The modelling also shows that the proposed future state of 3,200 pieces maximum WIP and 800 pieces batch size is able to fulfil overall customer demand and yields a customer service level well above 90 %. It further reveals that under the given framework, the settings result in the Lean optimum for the process, since lowering of either batch size or initial pull level gives a non-feasible process.

The lead time of the simulated future state was found to be 1.4 days average with 0.1 days standard deviation and 2.0 days maximum. Continuous rescheduling of shop floor process steps is made obsolete due to strongly reduced lead time from the original 11.4 days. New orders with close due dates can be channelled into the process without violating the FIFO rule with a maximum response time of two days.

The slightly higher lead time of the DES model compared to the static spread sheet simulation results from more realistic modelling, including process and customer demand variability, lunch breaks and simultaneous utilization of the belt oven for other product families.

The feasibility analysis model can also be used to predict the response of the future state process to changes of customer demand. Figure 41 and Figure 42 show the customer demand fulfilment in case of a 15 % demand increase. Both feasibility criteria show that the proposed future state is not able to fulfil the customer demand anymore. If changes in customer demand are expected, either technical process optimization projects have to be deployed or a different, more robust operational point has to be chosen. For potential 15 % demand increase in the case study, a capable process can be found at 1,500 pieces batch size and 6,000 pieces maximum WIP. This operating point leads to a Lean, yet robust process and should be implemented if customer demand is likely to increase and investment in technical improvement is to be circumvented.

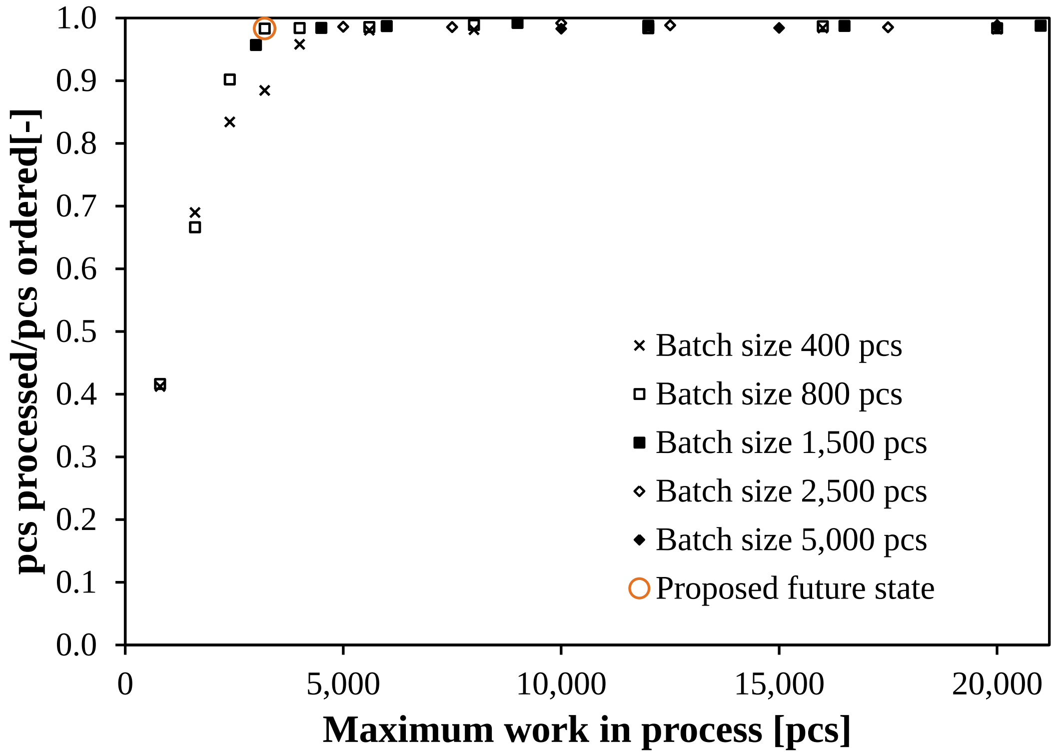


Figure 39: Case study 2 DES feasibility analysis – overall customer demand.

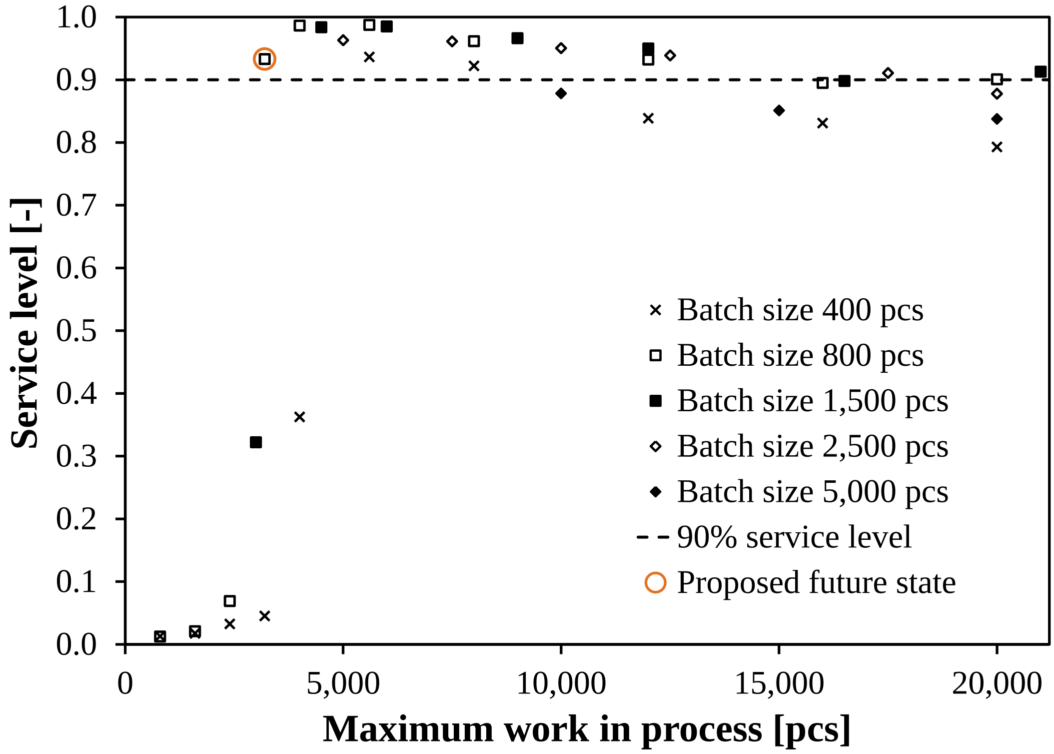


Figure 40: Case study 2 DES feasibility analysis – service level.

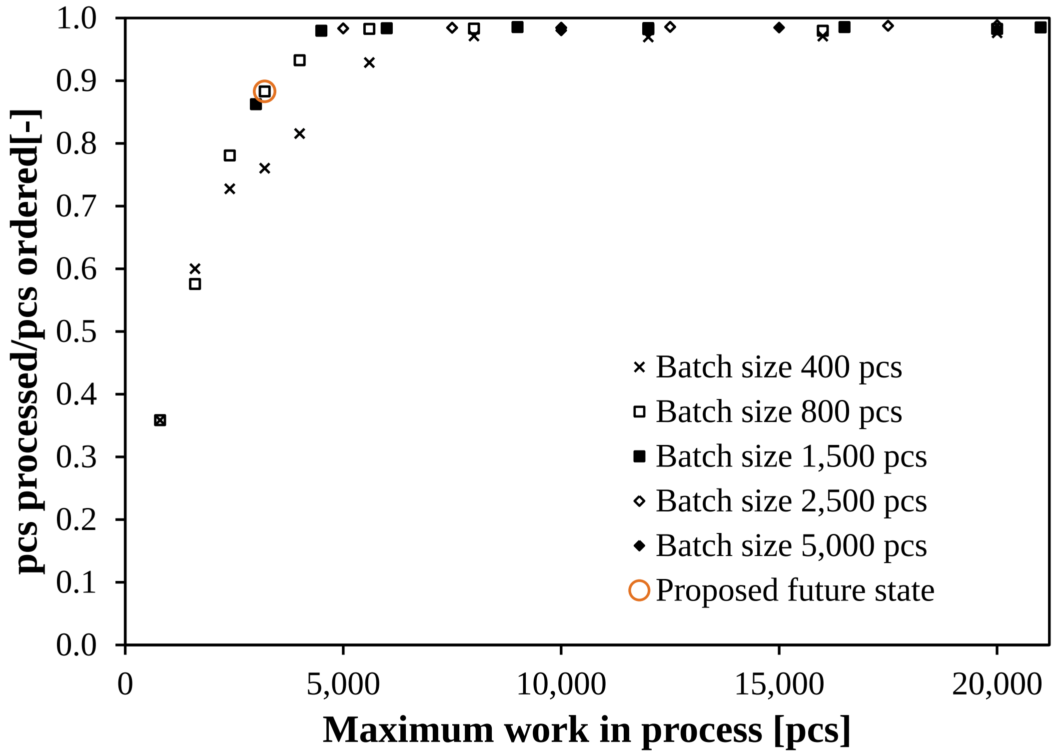


Figure 41: Case study 2 DES feasibility analysis – overall customer demand (15% demand increase).

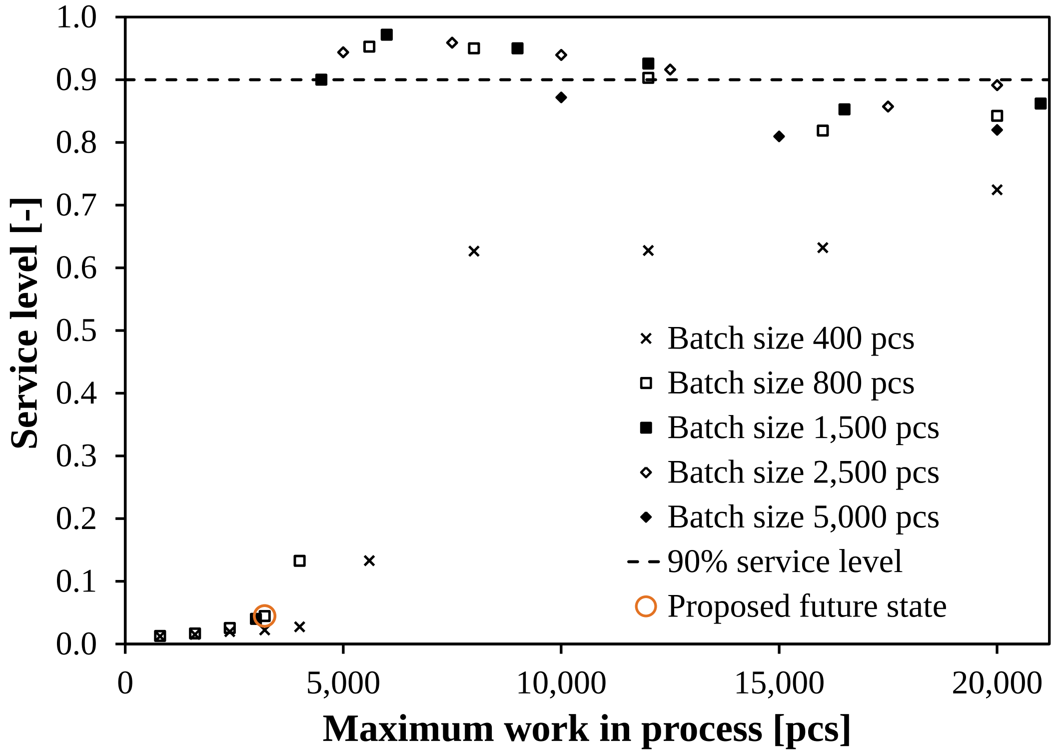


Figure 42: Case study 2 DES feasibility analysis – service level (15% demand increase).

5.2.4.3 Trade-off analysis.

In order to determine whether the proposed future state is beneficial when all affected cost components are considered, the DES model was further utilized for trade-off analysis. In the analysis, the parameters batch size and initial pull WIP level were varied. At the same time several cost components were observed and combined in an objective function:

- Cost of tied capital:

  The capitalization cost rate was calculated as 10 % p.a. for material inventory, which is a rather conservatively low number (Russel, 2012). The capitalization cost per product quantity is determined as a linear function of process lead time:

$$\left(\frac{cost}{q_p}\right)_{capitalization} = PLT \cdot \frac{10\ \%\ p.a.}{360\ d\ p.a.} \cdot \left(\frac{material\ cost}{q_p}\right) \qquad \text{Eq. 17}$$

- Scheduling effort cost:

  Due to the high inventory of the current state shop floor process, continuous scheduling effort for shop floor supervisors had been required. Thus, reduction of scheduling effort was identified to be a major effect of the VSM future state. Shop floor scheduling effort cost was modelled as a linear function of inventory and, through Little's law, of process lead time:

$$\left(\frac{cost}{q_p}\right)_{scheduling} = \frac{PLT \cdot daily\ demand}{\left(q_p\right)_{produced\ p.a.}} \cdot \left(\frac{scheduling\ cost\ p.a.}{\left(q_p\right)_{inventory}}\right) \qquad \text{Eq. 18}$$

- Cost of poor quality:

  Cost of poor quality was modelled as proposed by Rosenblatt and Lee (1986) as a function of batch size. The approach is based on the assumption that initially, after setup of a machine the production process is running with perfect quality. However after a certain amount of material, the process deteriorates and the defect rate α is observed. The amount of material, after which the process deteriorates is exponentially distributed with a mean value of $1/\mu$. The mean defect rate for the overall process can then be expressed as:

$$defect\ rate = \frac{\alpha \cdot \left(BS + \frac{1}{\mu} \cdot \exp(-\mu \cdot BS) - \frac{1}{\mu}\right)}{BS} \tag{Eq. 19}$$

For the case study process, the parameters α and 1/μ were fitted to the defect rate observed in the current state process over one year. From the defect rate, the cost per quantity produced can be calculated:

$$\left(\frac{cost}{q_p}\right)_{defects} = defect\ rate \cdot \left(\frac{material\ cost}{q_p}\right) \tag{Eq. 20}$$

– Energy costs:
  The predominant energy consumption of the process is rooted in the operation of the belt oven. It was therefore modelled as a linear function of the belt oven utilization time. The belt oven energy costs per time unit were based on consumption measurements and current natural gas prices.

$$\left(\frac{cost}{q_p}\right)_{energy} = \frac{energy\ cost\ per\ time \cdot belt\ oven\ utilization\ time\ p.a.}{\left(q_p\right)_{produced\ p.a.}} \tag{Eq. 21}$$

As expected, both tied capital as well as scheduling costs increase with increasing batch size and initial pull level, while energy costs decrease. Cost of poor quality increases with batch size while it is independent of initial pull level. The results of the overall objective function over the range of parameter settings is displayed in Figure 43. The proposed future state settings actually yield the overall cost optimum within the feasible options. However, as concluded from the feasibility analysis, the process is not robust towards customer demand changes. The trade-off analysis shows that there are various other operating points, which are feasible and at the same time cost efficient, especially compared to the current state. The operating point at 1,500 pieces batch size and 6,000 pieces maximum WIP suggested in the feasibility analysis, which is more robust towards customer demand increase for instance results in a beneficial process as well.

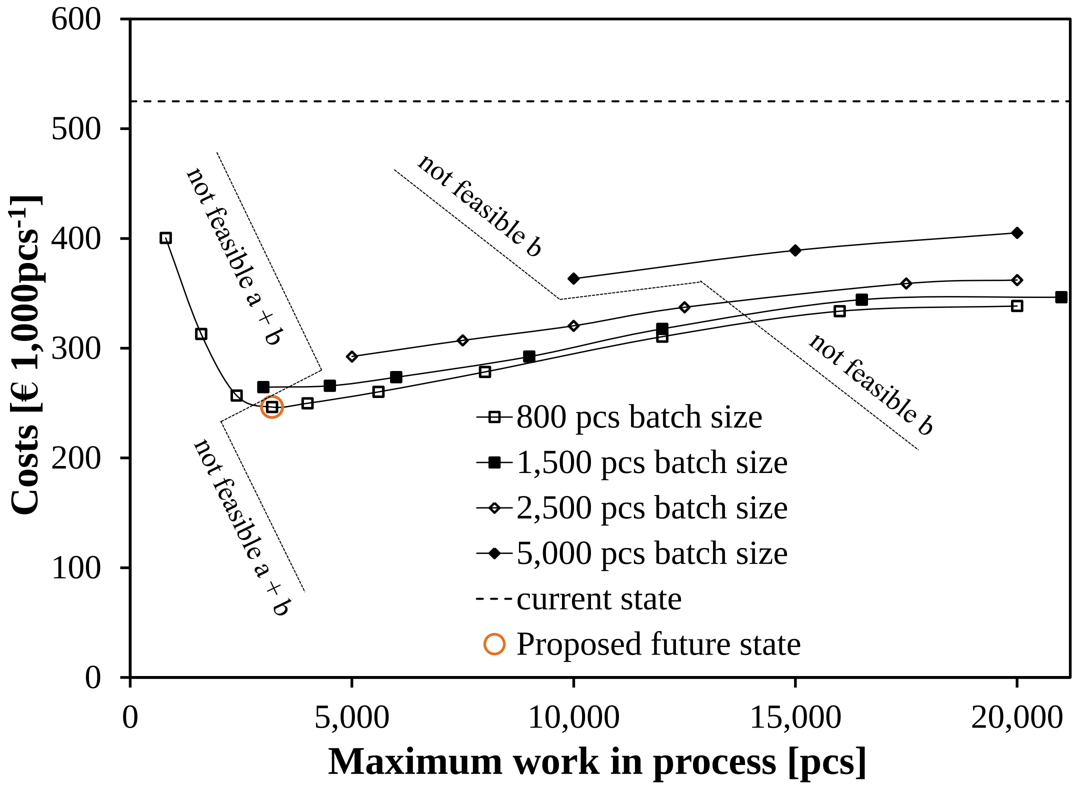


Figure 43: Case study 2 DES trade-off analysis. Separating lines indicate settings which are not feasible due to lack of fulfilment of overall customer demand (a) and service level (b).

5.2.5 Discussion

In case study 2, DES feasibility and trade-off analysis enhanced VSM was applied to a catalytic converter production process. The main issues tackled by the VSM project were high shop floor inventory, turbulence and scheduling effort. The VSM project was conducted up to development of the future state map as proposed by Rother and Shook (1999). Application of the VSM future state guidelines yielded a shop floor inventory reduction from 25,540 pieces to 3,200 pieces, based on static calculation. Furthermore, it was predicted that the shop floor scheduling effort could be reduced drastically.

Based on the current state and future state maps, a DES model was elaborated. The model was further refined by including process and customer demand variability. After verification and validation with the current state model, the future state model was utilized for feasibility and trade-off analysis. Feasibility analysis revealed that the proposed future state is capable of meeting the customer demand, however it is not capable in case the customer demand is increased by 15 %. With the future state model, it was possible to predict a slightly different future state capable of fulfilling a potentially increased customer demand. For trade-off analysis, capitalization cost, scheduling effort cost, cost of poor quality and energy cost were included. With the DES model and the cost components it was possible to quantify the benefit of various potential future states to each other and to the current state.

The case study proves the applicability of DES feasibility and trade-off analysis enhanced VSM. Applying the enhanced VSM method entails the following benefits for practitioners:

– Customer demand fulfilment is analysed prior to implementation, avoiding a potential iterative procedure, which is costly and, at the worst, leads to customer dissatisfaction.
– The actual monetary benefit of the proposed future state is determined before implementation. Consequently, the future state map can be refined, in order to obtain the most favourable process.
– DES results can be a precious tool for gaining management acceptance, as they provide hard figures instead of vague indication of the applicability and benefit.
– The original “paper and pencil” procedure of VSM, allowing straightforward involvement of process experts, is preserved.
– The effect of potential future changes in customer demand on the value stream optimized process can be predicted in advance.

Application of the feasibility and trade-off analysis requires additional effort. Original VSM projects can be carried out rather rapidly. Project durations between four and ten weeks have been reported (Serrano, Ochoa and de Castro 2008). For adding feasibility and trade-off analysis, relatively time-consuming process variability analysis and DES model building are required. For the case study, the additional procedure amounted to approximately four weeks. Furthermore, a simulation expert has to be involved in the project. Due to the user-friendliness of contemporary DES packages however, attaining simulation experts has become a less challenging issue.

Opposed to the low-detailed modelling of classical VSM, the enhanced method adds a considerable amount of complexity, inevitably creating pitfalls. Creating valid DES models demands detailed analysis of process parameters including their behaviour over time. Misinterpretation or lacking availability of process data can lead to false process input distributions for the DES model and ultimately to incorrect conclusions.

Developing a valid objective function involving all affected cost components for the trade-off analysis is particularly challenging. Detailed cost component modelling provides room for further research. In case study 2, four cost components directly affected by the VSM project were included. However, as shown in Figure 14 in Section 3.3, VSM may affect producer objectives in delay as well as market objectives, which can both not be included in an objective function straightforwardly. For this purpose there are several approaches supposable (see Section 2.3) which are worth exploring.

5.3 Case study 3: Application of DES/DRS for cost efficient operation of a precipitation/filtration unit

Case study 3 focuses on the application of the above introduced simulation tools as a decision support system for optimization of industrial chemical production. An exemplary three stage chemical process is implemented in an integrated DES, DRS and continuous simulation model. The model then serves as a basis for detailed process analysis and optimization, involving several cost components. While the optimization framework is similar as in the VSM projects discussed in case study 1 and 2, including similar optimization measures and cost components, case study 3 provides more details about the simulation approach instead of VSM project execution. Case study 3 is structured as follows:

First, the model process is introduced, the project is scoped and the problem is formulated. Thereafter, the project is presented in accordance with the structured simulation approach suggested by Banks et al. (2009) and outlined in Figure 17. Special attention is paid to model translation, where integration of the three simulation methods is elaborated, and model experimentation, where an Evolutionary Strategies algorithm is applied to find design parameter settings leading to a cost optimized process.

5.3.1 Process description and problem formulation

In the model process of case study 3, two different chemicals named product X and product Y are produced. The process is based on the following chemical reactions:

$$1A + 1B + 1D \rightarrow 1X \qquad \text{Eq. 22}$$

$$1A + 1C + 1D \rightarrow 1Y \qquad \text{Eq. 23}$$

The plant of the model process, outlined in Figure 44, is part of a chemical production site, where product X and product Y are consumed by a downstream process continuously but at varying rates. The four raw materials required are not available continuously, but are demanded batch-wise from an external supplier. Upon delivery, they are stored in four dedicated storage tanks. In the first of in total three processing stages, a chemical reaction takes place. For this stage, two batch reactors are available, one dedicated to each product. The intermediates produced in the two reactors are stored in individual buffer tanks. Subsequently the intermediates are precipitated, again in a batch process. For precipitation, only one vessel is available. From the precipitation vessel, the intermediates are fed to a filter press. The filter press is operated at constant pressure and, thus, varying volumetric flow rate. The filtrate represents the final product, while the filter cake is discharged. Only one filter press is available for both products. In the precipitation and filtration stages, product X and product Y are scheduled on an alternating basis. The final products are stored in individual buffer tanks, which serve as feed tanks for the downstream customer process.

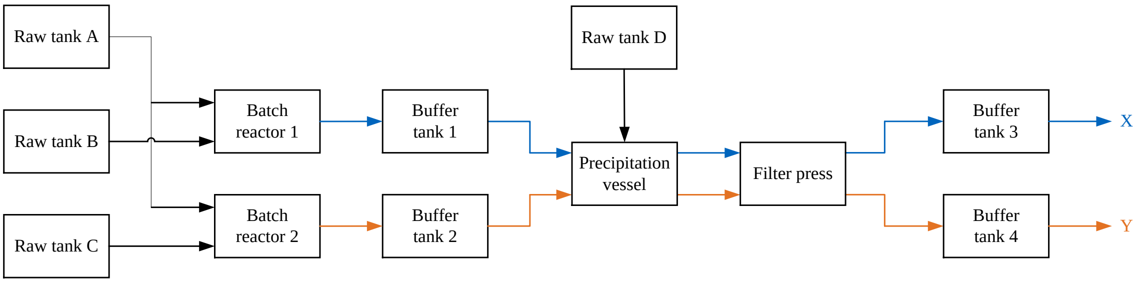


Figure 44: Process overview of case study 3 production.

The goal of the simulation study in case study 3 is to determine an operational mode of the process, leading to the lowest possible operating costs. The cost components affected by the optimization measures are summarized in Table 14.

Table 14: Cost components of case study 3 process.

Cost component	Unit	Value
Raw material delivery	€/delivery	1000
Raw material costs	€/unit[5] of raw material	3000 (A), 5000 (B), 2000 (C), 1500 (D)
Capitalization rate	% p.a.	10
Changeover of precipitation/filtration unit	€/cycle	1000
Cleaning of filter press	€/cycle	200
Operation of filter press	€/h	70
Revenue loss	€/unit of product	5000 (X), 3500 (Y)

In order to reduce the operating costs, two pull systems are suggested. The first pull system is proposed for the final products. When the final product buffer tank of either of the two products falls below a certain fill level (reorder point), production orders are sent to the precipitation stage for this product. The product is then produced until the fill level of the final product buffer tank reaches a defined upper limit (order termination point). Afterwards, operation of the precipitation unit is either stopped, or it is changed over to the other product in case the fill level of its buffer tank has meanwhile fallen below the reorder point. The second pull system concerns raw material supply and is proposed to follow a Q,r model. Fixed quantities of raw material are demanded from the suppliers only when the fill levels of the raw material tanks fall below a certain reorder point. For dimensioning of the pull systems, several options are available. These options, alongside other parameter settings which are changeable, are summarized in Table 15.

[5] The quantities of raw materials, intermediates and products throughout the process are generalized as ‘units’. The term ‘unit‘ as used in the following sections therefore represents a certain mass quantity.

Table 15: Changeable design parameters for cost optimization of case study 3 model process.

Design parameter	Available settings
Reorder points for precipitation stage (fill levels of final product buffer tanks)	10, 20, 30, 40, 50 or 60 % fill level
Order termination points for precipitation stage (fill levels of final product buffer tanks)	50, 60, 70, 80, 90 or 100 % fill level
Reorder points for raw materials (fill levels of raw tanks A,B, C and D)	Integer 9 – 149 units
Order quantity for raw materials	20, 40, 60 or 80 units
Allocation of four buffer tanks	The buffer tanks for intermediates and final products of 100, 200, 200 and 300 m³ can be arbitrarily changed
Volumetric flow rate below which filter press is cleaned	Integer 1 – 18 $m^3 h^{-1}$

5.3.2 Model conceptualization

A process flow diagram, serving as the basis for the simulation model and a detailed description of the process steps including input parameters are provided in Appendix A. For the simulation model, the process was structured into five subsystems (see Figure 45).

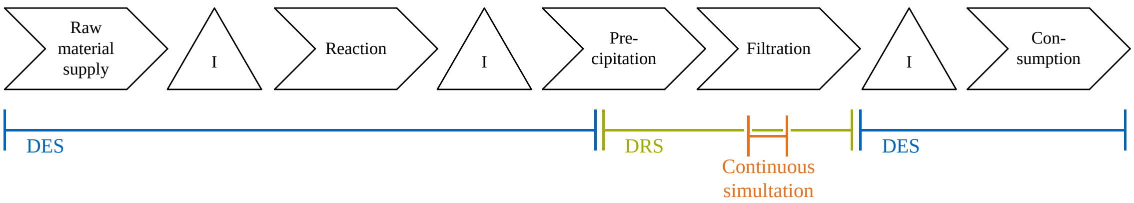


Figure 45: Simulation model subsystems and applied simulation techniques of case study 3 process.

Raw material supply is modelled with DES. One unit of raw material is represented as one entity in the model. For each raw material, entities are created batch-wise with the predefined order quantity whenever the inventory queue downstream of raw material supply falls below the respective reorder point. Reaction is as well modelled with DES. Here, one entity of raw A is merged with one entity of raw B (for product X) or raw C (for product Y) into one entity representing a unit of intermediate X or Y. The reaction itself is represented as a delay process with varying durations per entity (see Table 16). The process is initiated whenever both raw materials are available in the upstream inventory queue and capacity is available in the downstream buffer tank queue. Both DES and DRS is applied for the precipitation subsystem. One entity of either intermediate X or intermediate Y is channelled through a DES delay process step, before it is transformed into 10 m^3 of DRS flow material. The precipitation process, with varying processing time (see Table 16) is initiated whenever replenishment orders are provided by the final product inventory queues downstream of the filtration unit, the respective intermediate material is available and the filtration unit is not occupied. When a changeover order is sent by the final product inventory queues, the process is disabled for the predefined changeover time. The filtration unit is modelled as continuous simulation integrated DRS. The filter press is modelled as a DRS valve. Due to the fact that the flow rate continuously decreases with the accumulation of filter cake, it has to be continuously updated. This is done by a filter equation for accumulated volume dependent volumetric flow rate at constant pressure, taking into account both resistance of the filter medium and specific resistance of the filter cake (see Appendix A for details). Filtration takes place whenever flow material is available from the precipitation unit. The unit is disabled for the predefined cleaning time whenever the volumetric flow rate falls below the minimum allowed. Finally, product consumption is again modelled as DES. Each DRS flow quantity of 10 m^3 is converted to an entity representing one unit of final product X or Y, before it is stored in the product buffer tanks modelled as DES queues. Consumption itself is modelled as a delay process with varying duration (see Table 16), after which entities are terminated.

Table 16: Variability distributions of case study 3 simulation model.

Process parameter	Distribution type	Most likely	Minimum	Maximum
Process time batch reactor 1 [h]	triangular	12	8	16
Process time batch reactor 2 [h]	triangular	10	7	20
Process time precipitation vessel 2 [h]	triangular	3.0	1.5	4.5
Consumption time product X [h/unit]	triangular	24	16	32
Consumption time product Y [h/unit]	triangular	16	10	22

5.3.3 Model translation and verification

The simulation model as conceptualized above was implemented in ExtendSim® AT, using elements of the program's Value, Item and Rate library. Implementation of the DES subsystems was achieved rather straightforwardly. For more information on DES model building with ExtendSim®, see Diamond et al. (2013). Verification of the DES subsections involved tracing of process flow, animation of the model and trend analysis of various aspects of the model. Figure 46 for instance shows the trend of the DES queue representing the raw tank A. In the graph, characteristics as expected for a Q,r pull system can be observed.

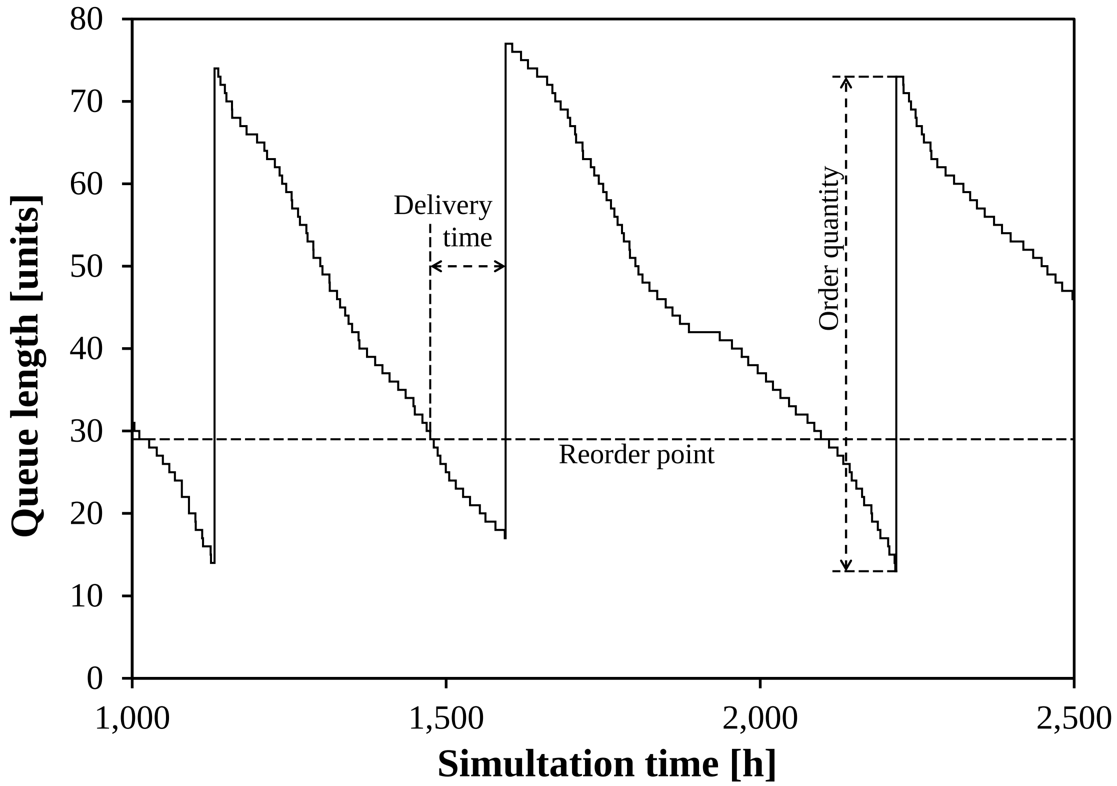


Figure 46: Queue length of raw tank A in case study 3 simulation model. Reorder point = 29 units, order quantity = 60 units.

Modelling the continuously changing rate of the filtration section was approached as introduced in Figure 22 (Section 4.3.3). It was found that modelling the volumetric flow rate of the filter press exclusively with discrete simulation was not an option, as the outcome would significantly differ from the real process. It was further found that tracing of the material balance through the model was not required. The solid content of the filtration feed remains constant over time and, thus, the only flow inherent attribute that affects the filtration rate is accumulated volume. The concept for integrating continuous simulation into the model for the filtration subsystem is illustrated in Figure 47. The time increment of the continuous model (Δt) was set to 0.05 h, as no significant effect on the simulation results of further lowering it was observed.

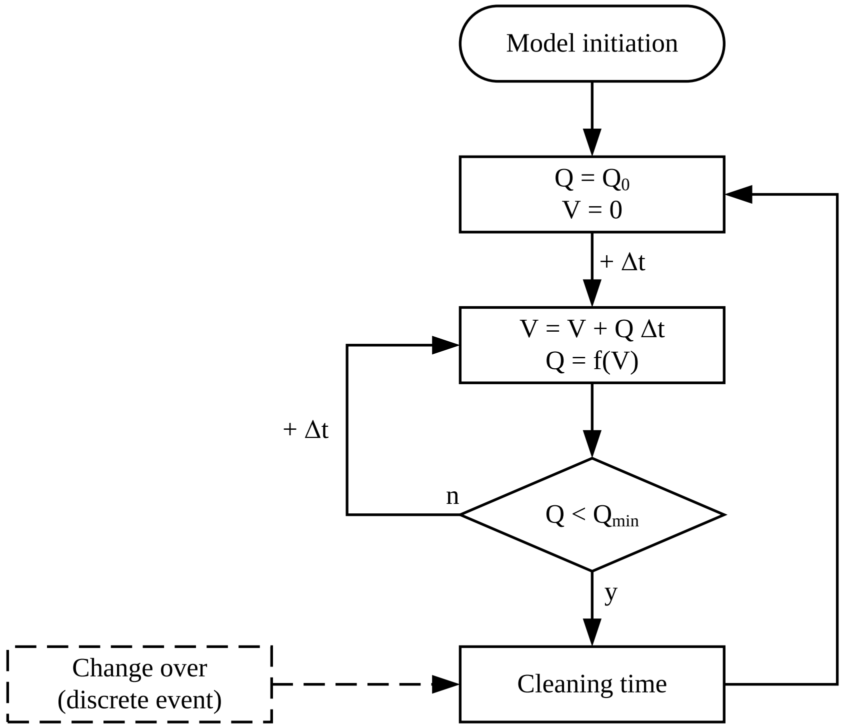


Figure 47: Concept for modelling the filtration subsystem of case study 3 with continuous simulation. Q is volumetric flow rate and V is accumulated volume.

For verification of the filtration subsystem, the simulation results were compared to the analytical solution of the filtration model. With volumetric flow rate being the derivative of accumulated volume over time, it calculates with the following ordinary differential equation (cf. Appendix A):

$$\frac{dV}{dt} = \frac{1}{a_1 \cdot V + a_0} \qquad \text{Eq. 24}$$

The equation is solved as:

$$V(t) = \frac{-a_0 + \sqrt{{a_0}^2 + 2 \cdot a_1 \cdot t}}{a_1} \qquad \text{Eq. 25}$$

Comparison of the simulation results with the analytical solution, which are in good agreement, is provided in Figure 48.

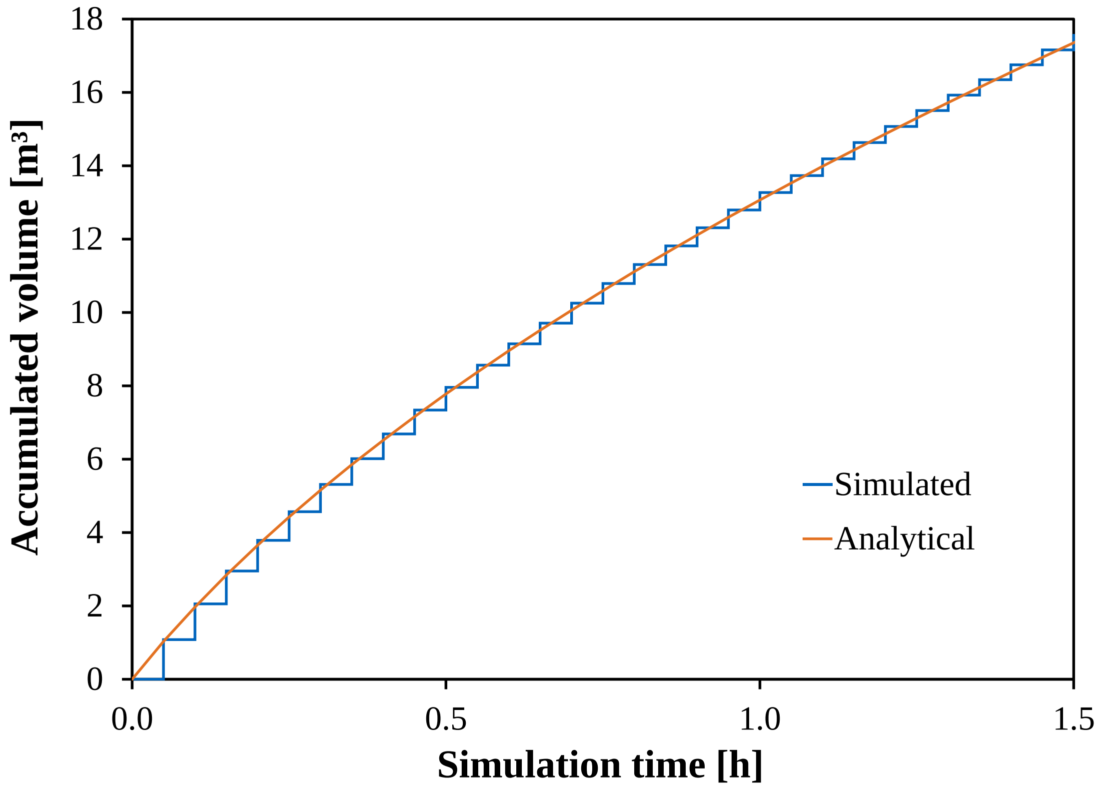


Figure 48: Comparison of simulation results for filtration subsystem of case study 3 with analytical solution.

5.3.4 Model experimentation and analysis

After implementation of the simulation model, cost optimization was tackled via simulation experimentation. The simulation duration was set to 4000 h per run, leading to a sufficient number of cycles of raw material deliveries, changeovers and filter press cleanings. Since the simulation model was initiated without work in process, the initial transient phase prior to stabilization of the process had to be eliminated. For this purpose, another 1000 h simulation duration were added to the beginning of the simulation model, of which the simulation results were discarded. For evaluation of the simulation results, the cost components summarized in Table 14 were transformed into an objective function, which can be found in Appendix A.

The changeable design parameters as summarized in Table 15 yield a solution space of $1.16 \cdot 10^{19}$ feasible options to configure the process. The number of simulation runs required to explore the full solution space even exceeds this number as the model is non-deterministic and multiple runs are required per option to obtain simulation results with a certain confidence level. In order to reduce the number of simulation runs required to find the optimum set of parameter settings as far as possible, simulation optimization was applied. An Evolutionary Strategies (ES) algorithm was chosen for rapid optimum search within the solution space. ES is a heuristic approach to find optimal or near-optimal solutions by imitating the principles of natural evolution (Carson and Maria 1997). A comprehensive introduction to ES is provided by Beyer and Schwefel (2002). The procedure within the algorithm is elaborated in Figure 49. The algorithm evolves with multiple iterations, which in analogy with biological evolution are termed ‘generations’. Each generation consists of a specific number of ‘parents’, i.e. cases with different parameter settings, from which ‘offspring’, i.e. new cases, evolve. Determination of a new generation comprises the three elements ‘recombination’, ‘mutation’ and ‘selection’, which are also found in natural evolution. While recombination and mutation aim for exploration of the solution space, selection facilitates exploitation of the most promising parameter settings. Usually, the following notation is used for ES algorithms:

$$\left(\mu/\rho \overset{+}{,} \lambda\right) \qquad \text{Eq. 26}$$

where μ is number of parents per generation, ρ is mixing number and λ is number offspring per generation.

The parameters μ, ρ and λ are called ‘exogenous strategy parameters’ which are kept constant during the evolution run. In addition there are several ‘endogenous strategy parameters’, such as probability of mutation, which may be changed through self-adaption during the evolution run (Beyer and Schwefel 2002). For selection of the next generation of parents, there are two procedures available. The next generation is either selected from parents and offspring of the previous generation (notation: (μ/ρ+λ)) or only from the offspring of the previous generation (notation: (μ/ρ,λ)). For termination of ES algorithms, commonly used conditions are maximum number of generations, maximum cpu-time or convergence of objective function results.

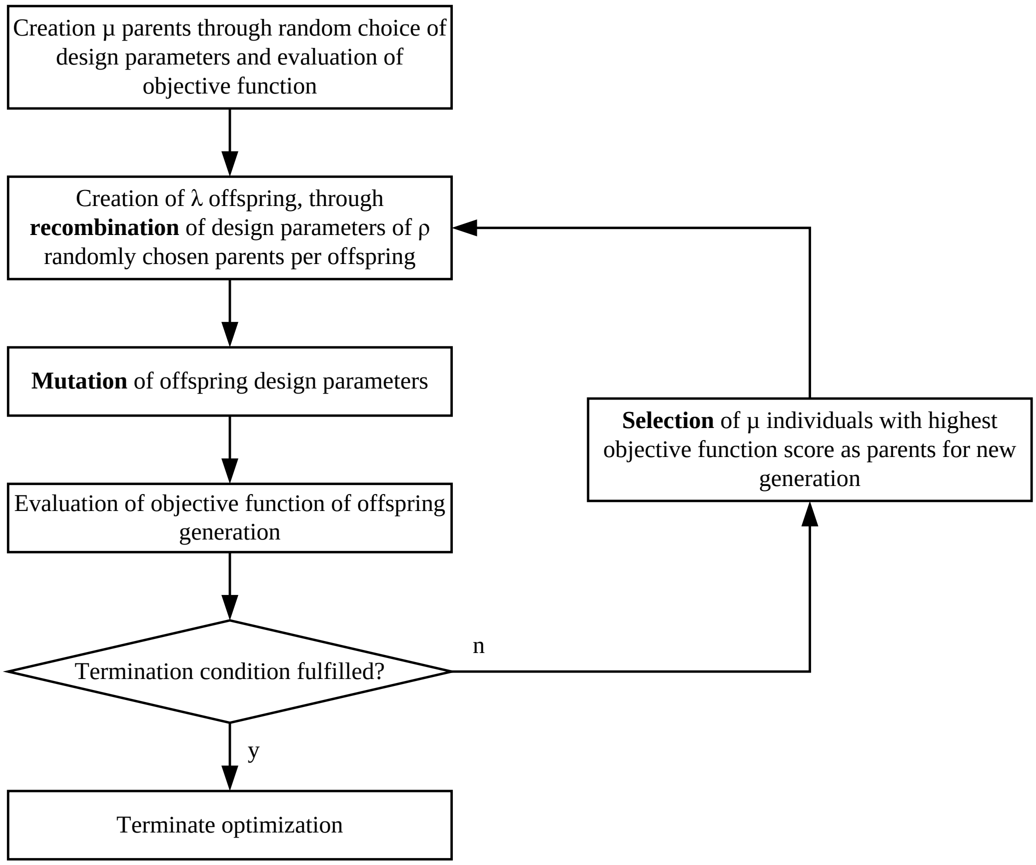


Figure 49: Basic concept of Evolutionary Strategies algorithms.

The ES algorithm applied within the ExtendSim® case study model evolves with $\lambda = 1$ offspring per generation. Recombination is performed by mating $\rho = 2$ parents. The first parent is the population member with the highest objective function score. The second parent is selected through tournament selection (Miller and Goldberg 1995) from the remaining population members. New generations are selected from parents and offspring. Further parameters of the algorithm as applied in the case study are summarized in Table 17.

Table 17: Parameter settings of ES algorithm applied in case study 3.

ES parameter	Setting
Member population size μ	10 cases
Number of simulation runs per case	10 runs
Termination condition	convergence of population (best and worst within 99.7 %)
Earliest termination	after 100 cases
Latest termination	after 1000 cases

Application of the ES algorithm to the case study process resulted in a cost minimum of 120,000 € $(4000\,h)^{-1}$, found after 293 generations. In order to verify whether the algorithm is able to determine the global cost optimum within the solution space, it was run several times. As only slight variations of cost minimum and design parameter settings were observed, effectiveness of the algorithm was concluded. The optimized design parameters determined by the ES algorithm are summarized in Table 18. Evolution of the objective function as well as its convergence within the population is shown in Figure 50.

Table 18: Design parameter settings of case study 3 optimized by ES algorithm.

Design parameter	Setting
Reorder points for precipitation stage (fill levels of final product buffer tanks)	30 % (X); 10 % (Y)
Order termination points for precipitation stage (fill levels of final product buffer tanks)	70 % (X); 90 % (Y)
Reorder points for raw materials (fill levels of raw tanks A,B, C and D)	9 units (A); 9 units (B); 13 units (C); 11 units (D)
Order quantity for raw materials	80 units (A); 40 units (B); 60 units (C); 80 units (D)
Allocation of four buffer tanks	tank 1: 10 m^3; tank 2: 20 m^3; tank 3: 20 m^3; tank 4: 30 m^3
Volumetric flow rate below which filter press is cleaned	5 $m^3\,h^{-1}$

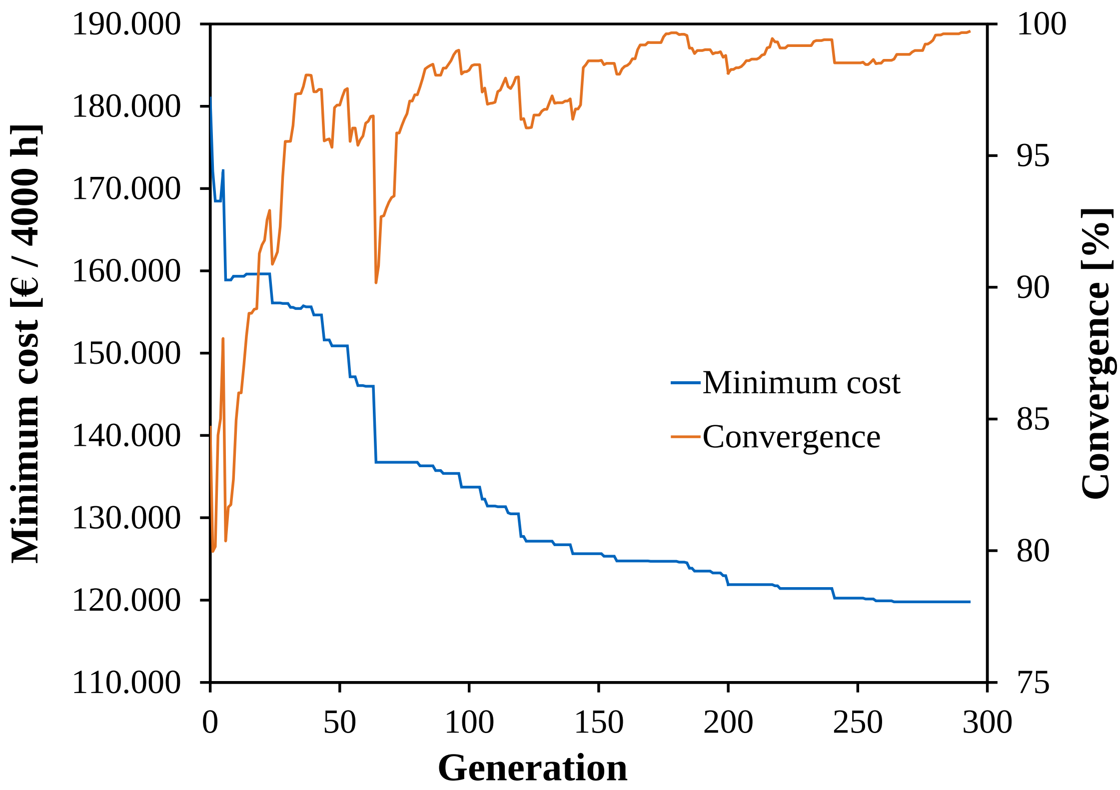


Figure 50: Objective function results of case study 3 ES algorithm.

The optimum design parameter set was further validated by multiple simulation runs, leading to a relative error 0.5 % at a 99 % confidence level for the objective function result. The simulation campaign resulted in a minimum cost of 121800 € $(4000\ h)^{-1}$ with an absolute error of ± 600 € $(4000\ h)^{-1}$.

Additionally, the reorder points of raw materials, as found by the algorithm, were recalculated as outlined by King (2009) for optimal Q,r model supermarket design. Here, the reorder point calculates as

$$reorder\ point = DDLT + safety\ stock \qquad \text{Eq. 27}$$

where DDLT is demand during lead time.

DDLT is calculated from the raw material lead time – the time lag between raw material ordering and raw material arrival – multiplied by the average demand rate for the respective raw material. Safety stock calculates as:

$$Safety\ stock = z \cdot \sqrt{\frac{RMLT}{T1}} \cdot \sigma \qquad \text{Eq. 28}$$

where σ is standard deviation, z is number of standard deviations, T1 is the time interval from which the standard deviation is calculated and RMLT is raw material lead time.

In Eq. 28, the standard deviation represents the variability in demand of the respective raw material. The number of standard deviations determines the cycle service level (i.e. the percentage of ordering cycles during which statistically the safety stock should prevent from running out of raw material). For the case study, $z = 3.09$ was chosen, entailing a cycle service level of 99.9 %. The standard deviation of demand was obtained from simulation experiments of $T1 = 1000$ h. The results of the Q,r reorder point calculation for the four raw materials are summarized in Table 19. As can be seen from comparing Table 19 to Table 18, the calculated reorder points and the reorder points obtained from the ES algorithm are in rather good agreement. Simulation experiments with the calculated reorder points yielded a minimum cost not significantly differing from the minimum cost obtained from the ES algorithm.

Table 19: Q,r reorder point calculation for case study 3 process.

Raw material	Relevant products	σ [units]	RMLT [h]	Demand rate [units h^{-1}]	DDLT [units]	Safety stock [units]	Reorder point [units]
A	X + Y	1.56	120	0.104	12.5	1.7	14.2
B	X	0.98	240	0.042	10	1.5	11.5
C	Y	1.21	192	0.063	12	1.6	13.6
D	X + Y	1.56	120	0.104	12.5	1.7	14.2

5.3.5 Discussion

Case study 3 focused on the application of DES for optimization of chemical production processes, a field which is only scarcely covered in academic literature. Emphasis was in particular put on explication of the DES model itself as well as experimentation with the model.

The DES model built for the three-stage chemical production process of the case study comprises subsections of both DRS and continuous simulation. DRS was capable of accurately modelling the discontinuous bulk flow processes through the buffer tanks and the precipitation tank of the model. Coupling of the discrete simulation techniques with continuous simulation gave the opportunity to implement the continuously changing filtration rate in the model. The case study suggests that combination of all three simulation types provides a promising toolset for adequately modelling complex transient chemical processes.

Experimentation was performed with the aid of the heuristic optimization technique Evolutionary Strategies, integrated in the simulation software ExtendSim®. Heuristic optimization techniques have been identified as efficient tools for experimentation with DES models (cf. Carson and Maria 1997 or Law 2007). In the case study, the ES algorithm was successfully applied to a combined DES, DRS and continuous simulation model. The algorithm led to efficient determination of a beneficial set of design parameters with a number of experiments representing only a fraction of the solution space. The design parameter settings for reorder points of raw materials suggested by the ES algorithm were recalculated by the method for supermarket design of Q,r pull systems outlined by King (2009). Concurrence of the cost minimum obtained with both methods suggests that the ES algorithm was able to find optimal or at least close to optimal design parameter settings.

Even though the case study indicates the benefit of combined DES, DRS and continuous simulation for modelling and optimizing transient chemical processes, there is considerable room for further research. Since the case study covered a model process, the rather complex subject of process data collection and modelling of these data as simulation input was unnecessary. Furthermore, in the continuous simulation subsection of the model, tracing the material balance was not relevant, as the solid content of the filtration unit feed remained constant over time. Tracing the composition of flow material in particular through discrete simulation models is challenging. Another area representing room for further research is design of the optimization objective and its implementation in an optimization algorithm. In the case study, a manageable amount of objectives could be translated into cost components and channelled into a uniform objective function. However, optimization objectives may be more versatile, for instance in VSM projects. On the one hand there may be additional cost components involved, in case study 3 for instance cost of poor quality as a function of campaign length of the two products, or cost of maintenance as a function of filter cleaning cycles. Here, finding a valid relationship to design parameter settings represents the major challenge. On the other hand, there may be optimization objectives which cannot be directly translated into cost components (delayed producer objectives or market objectives, cf. Figure 14). Here formulation of a uniform objective function is a complex task and provides room for further research.

5.4 Case study 4: Application of DES/DRS for debottlenecking of a complex multi-stage waste water treatment process

Case study 4 covers the application of DES, DRS and continuous simulation for debottlenecking of a complex chemical process. The process, which stretches over three individual plants, comprises the waste water treatment of an upstream process including byproduct isolation. Similar to case study 3, case study 4 emphasizes on evaluating the usefulness of the simulation tools for optimization of chemical processes. In particular, focus is put on simulation input parameter modelling and implementation of the simulation model itself.

As in case study 3, presentation is structured in accordance with the approach suggested by Banks et al. (2009) outlined in Figure 17. After description of the process, the conceptual model is elaborated, translation of the simulation model is explicated and experimentation and analysis with the model is provided.

5.4.1 Process description and problem formulation

The task of the production process of case study 3 is waste water purification of an upstream process as well as separation of an inorganic salt as byproduct. The process comprises numerous continuous and discontinuous unit operations and ranges over three different plants, which are depicted in Figure 51 and outlined in the following paragraphs:

– *Precipitation plant:*

  Upstream production processes provide a precipitation plant with a salt solution contaminated with various metals. In a batch process, the metals are precipitated. The emerging slurry is then channelled through a filtration unit. While the filter cake is discarded, the filtrate is passed through several other purification units. The precipitation plant consists of two parallel processing lines, a line high in byproduct concentration (HC line) and a line low in byproduct concentration (LC line).

– *Reverse osmosis plant:*

  The purified solution from the precipitation plant is consecutively fed to a reverse osmosis (RO) plant. In this plant, the byproduct is concentrated in five interlaced RO steps. While the solvent partly permeates through the membranes, the product is completely detained in a concentrated solution.

– *Evaporation plant:*

  The concentrated solution is then passed to an evaporation plant. Here, the solvent is evaporated while the byproduct crystalizes. The process step takes place in two evaporator units operated in series. After evaporation, the byproduct is freed from residual solvent in a hydrocyclone, a centrifuge and a belt dryer. Finally, the byproduct is packaged and transferred to a storage area for shipping.

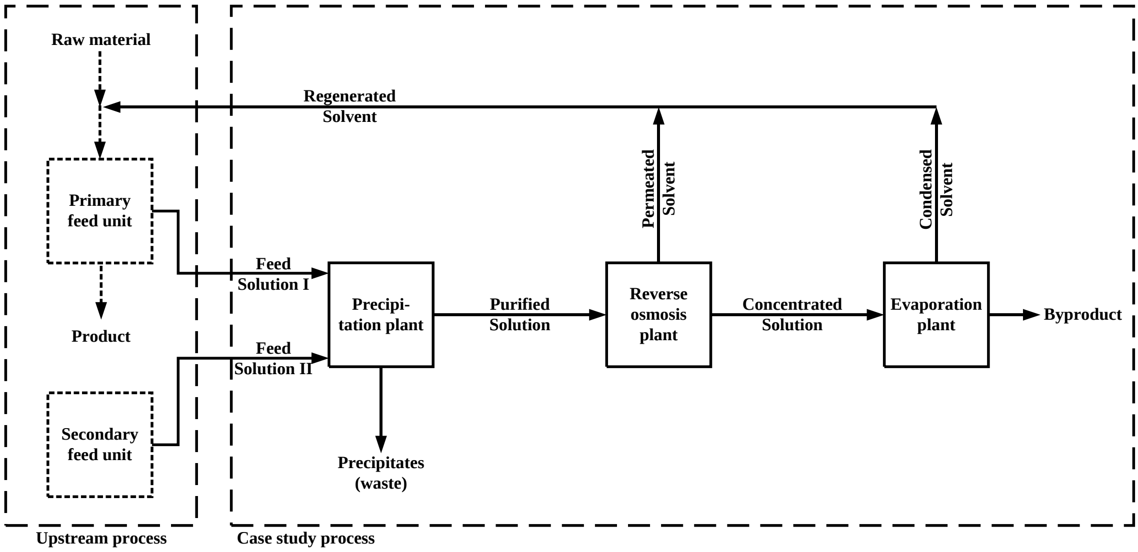


Figure 51: Overview of case study 4 chemical production process

The feed of the case study process originates in several other production processes, as well as discontinuous recycling of the process itself. The dominating share of feed is the liquid fraction of an upstream precipitation process (primary feed unit). As this process is operated in batch mode, the feed is available discontinuously. Feed is generated during mother liquor filtration, as well as several washing steps. The pattern of the feed arrival process from the primary feed unit is shown in Figure 52. After a period of variable duration required for several, non feed generating actions, the first part of the mother liquor filtrate is fed to the HC line of the precipitation plant. Consecutively, the second part of the mother liquor filtrate, as well as the filtrate of the washing steps is fed to the LC line. Under normal operation, the upstream process is able to generate feed at a higher rate than the purification process can consume. Thus, under steady state conditions, the purification process in focus of case study 4 represents the global bottleneck.

The mother liquor and the individual washing steps of the primary feed unit as well as the secondary feed units generate solutions with different byproduct concentrations. This effects varying concentrations within the plants of the case study process, depending on the origin of its feed.

The units of the case study process are partly batch wise and partly continuously operated. As the feed is supplied in batches, the precipitation plant is operated discontinuously. The more downstream RO and evaporation plants on the other hand employ continuous processing. This is facilitated by several buffer tanks between the three plants.

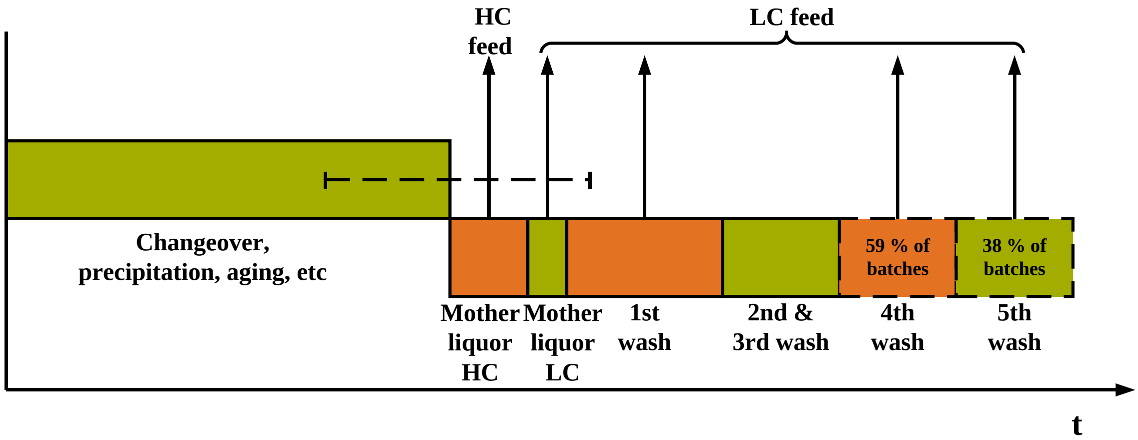


Figure 52: Pattern of waste water generation of a production batch in the primary feed unit of case study 4 (dashed lines indicate process variability).

5.4.2 Model conceptualization and input parameter modelling

The flow diagram of process steps as they were broken down for the simulation model is presented Figure 63 in Appendix B.1. Process data serving as the basis for the simulation model are provided in Appendix B.2

As the overall process comprises batch units, as well as continuously operated units, decisions had to be made where to apply DES and where DRS. For the primary feed unit as well as the secondary feed units, the most important information was time between batch arrivals and feed volume per batch. For modelling these processes, DES was found to be the most suitable approach. From the precipitation plant onwards, DRS was chosen in order to model the flow of bulk material adequately. Downstream of the evaporation plant, for packaging and dispatching of the byproduct, again DES was selected because discrete items (i.e. packages of byproduct) are handled. In that way, only two interfaces between DES and DRS are created. From the discrete feed units, bulk flow material is released into the precipitation plant. Between the precipitation plant and the evaporation separation step (cf. Figure 63) the DRS flow media represents volume of solution. Downstream of the evaporation separation step, for the hydrocyclone, the centrifuge and the belt dryer, the flow media is converted into mass of byproduct as a function of evaporation feed volumetric flow rate and evaporation feed concentration, before it is converted into discrete packages of byproduct.

In order to model the process adequately, data gathering was initiated. For this purpose, production records were evaluated, Subject Matter Experts were interviewed and selected process parameters were monitored. It was found that the case study process comprises several sources of variability, distributed over all three plants as well as the feed processes. Deviation of the process from steady state had multiple reasons which can be structured into two types of variability:

– Random variability:

  Random failures of processing units resulted in deviation from the steady state of the case study process. A significant density of random shutdowns due to failure was found for the precipitation plant, the evaporation plant and dispatching of the byproduct. Randomness was observed for the time between failures as well as the failure duration. Another source of random variability was found in the primary feed unit with time between batch arrivals and in the secondary feed units with time between batch arrivals as well as volume per batch. For the purpose of integrating these sources of randomness into the simulation model, probability distributions were selected using the statistical software package Stat::Fit®. First, sample independence was assessed and could be proven through correlation plots. Distributions were then fitted to the process data using Maximum Likelihood estimation. Finally, a probability distribution for the simulation model was selected with the Anderson Darling test, supported by graphical comparison of process data histograms to the individual probability distributions. Details about the probability distributions chosen for the case study process can be found in Appendix B.2.

  Another type of random variability was observed in the primary feed unit with the number of washing steps per batch. The final two washing steps were only required with a certain probability (see Figure 52). It was found that the number of washing steps was strongly autocorrelated across batches. In other words, the probability that five washing steps were required was significantly higher if the previous batch had also required five washing steps than if the previous batch had required three or four washing steps. In order to simulate the probability for number of washing steps fittingly, a third order Markov chain model was elaborated for the decision whether the fourth washing step is required. The decision whether the fifth washing step is required was simulated with a second order Markov chain model. Details about the Markov chain models including their transition matrices are provided in Appendix B.2.

– Correlated variability:

  Random variability of input and process parameters effected deviation of additional parameters from steady state. This correlated variability was either an effect of operator decisions or physical law. The former was found for the feed rates of the RO plant and the evaporation plant, as well as ratio between HC and LC feed of the RO plant. Decisions for changing these parameters were made based on the fill level of the feed tanks of the corresponding processing unit. The specific mechanisms as derived from operator interviews and parameter monitoring can be found in Appendix B.2. Correlated variability based on physical law was found for the separation ratio of the RO plant and the evaporation plant. The separation ratio between concentrate and permeate of the RO plant was found to be a function of HC and LC feed rate as well as HC and LC feed byproduct concentration. The relationship between the feed parameters and the RO separation ratio was determined through multiple linear regression analysis. The resulting equation used for the simulation model can be found in Appendix B.2. The separation ratio of the evaporation plant was a simple function of byproduct concentration, as the byproduct was fully isolated from the solvent.

5.4.3 Model translation, verification and validation

Based on the conceptual model, the ExtendSim® simulation model was built. All the DES and DRS sections were modelled with the aid of the simulation package as introduced in Section 4. Random variability and correlated variability as an effect of operator decisions were as well modelled with the discrete simulation techniques, as they affected the process at discrete points in time. Correlated variability as an effect of physical law on the other hand had a continuous effect on the process. Through the random variability of the feed processes, the byproduct concentration of the feed of the precipitation plant changes at discrete points in time. However through backmixing in the tanks of the precipitation plant, the concentration changes continuously further downstream. As an effect, the separation ratio of the RO plant and the evaporation plant changes continuously as well. Modelling these continuously changing attributes adequately therefore entailed tracing of the full material balance through the case study process, which is elaborated as option III in Figure 22 (Section 4.3.3).

Tracing the material balance of transient flow within a system of interconnected tanks analytically requires setting up and solving of interconnected differential equations. Consider for instance the rather elementary case displayed in Figure 53. A continuously stirred tank initially filled with a certain volume of solvent and specific product concentration is filled continuously with solvent with constant flow rate and constant product concentration. At the same time, the tank is emptied with constant flow rate.

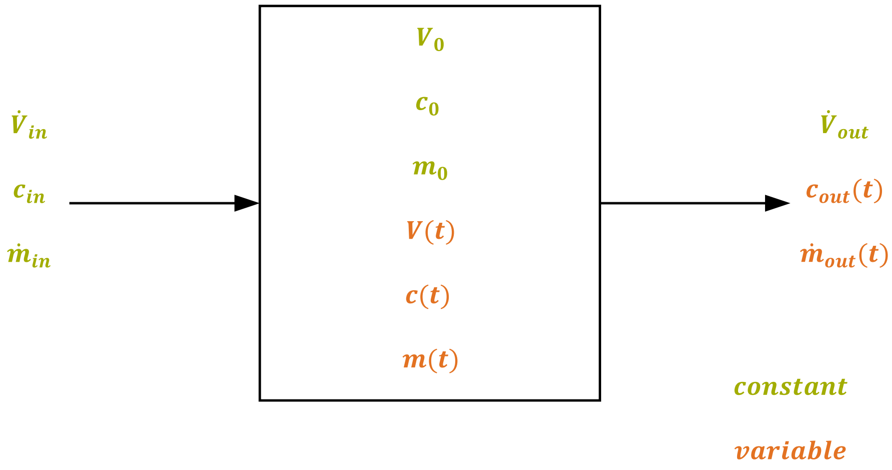


Figure 53: Elementary case of material balance tracing through a continuously stirred tank.

In order to trace the mass of product present in the tank over time, and thereby its concentration, the following first order linear differential equation needs to be solved:

$$\frac{dm}{dt} + \frac{\dot{V}_{out}}{V_0 + (\dot{V}_{in} - \dot{V}_{out}) \cdot t} m(t) = \dot{m}_{in} \qquad \text{Eq. 29}$$

The particular solution calculates as:

$$m(t) = \frac{1}{\dot{V}_{in}}\dot{m}_{in}\left(\left(\dot{V}_{in} - \dot{V}_{out}\right)t + V_0\right) + \left(m_0 - \frac{V_0\dot{m}_{in}}{\dot{V}_{in}}\right)V_0^{\frac{\dot{V}_{out}}{\dot{V}_{in}-\dot{V}_{out}}}\left(\left(\dot{V}_{in} - \dot{V}_{out}\right)t + V_0\right)^{-\frac{\dot{V}_{out}}{\dot{V}_{in}-\dot{V}_{out}}} \quad \text{Eq. 30}$$

In case of a system of multiple tanks in line, the analytical solution becomes significantly more complex, than in the exemplified elementary case, due to the fact that the feed concentrations of the individual tanks are inconstant because of backmixing inside the respective upstream tanks. However, integrating exact material balance tracing into a DES or DRS model requires solutions to the arising differential equations and their evaluation at each discrete event recalculation point.

This effort can be avoided with the simplifying assumption of plug flow between recalculation points and backmixing only at discrete events. An example for this two-stage procedure is shown in Figure 54. Application of the procedure, however, entails deviation from the exact solution, which for the example of Figure 54 is provided in Figure 55. This deviation increases with increasing time lag between discrete events and concentration difference among connected tanks.

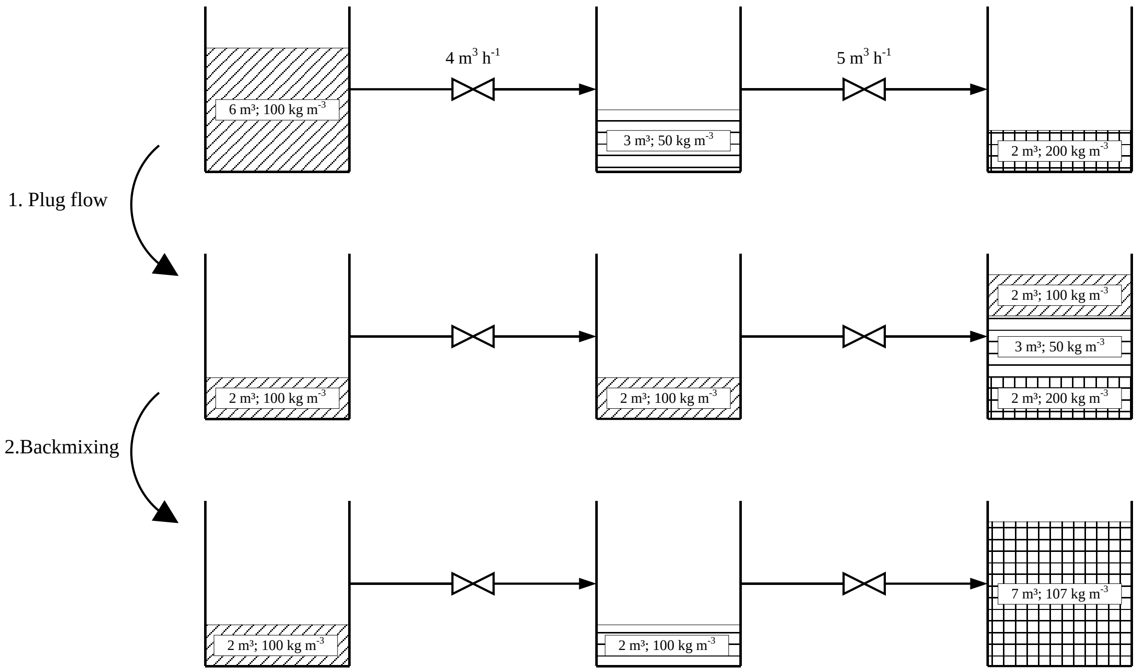


Figure 54: Simplifying two-stage procedure for tracing the material balance of dissolved product through a DES/DRS model. Time lag between recalculation points: 1 h.

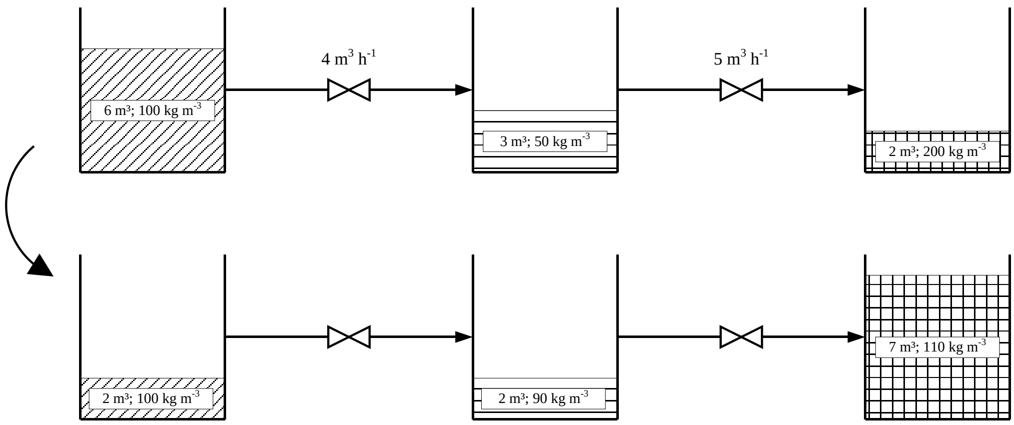


Figure 55: Exact solution to the example of Figure 54 for tracing the material balance of dissolved product through a DES/DRS model. Time lag between recalculation points: 1 h.

An improvement of the two-stage procedure can be gained by introducing additional recalculation points to the model. At the expense of model execution time, continuous recalculation of the material balance in addition to the discrete recalculation points (see Figure 56) leads to convergence towards the exact solution. It further provides the option to synchronize recalculation of downstream process steps depending on product concentrations with the material balance recalculation points, and thereby increases their accuracy.

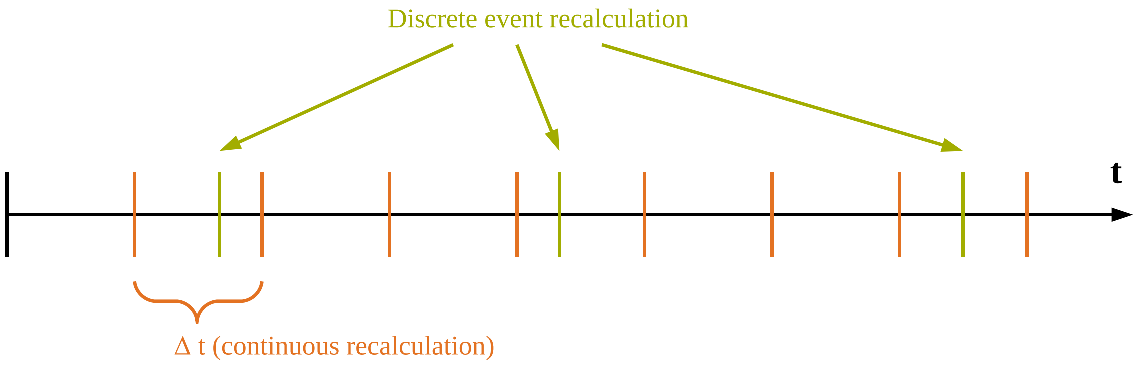


Figure 56: Continuous and discrete material balance recalculation points in case study 4 simulation model.

The two-stage material balance recalculation procedure with additional continuous recalculation points was selected for modelling the process of case study 4. The algorithm of its implementation in the ExtendSim® model, which is valid for both, the procedure with and without continuous recalculation points, is elaborated in Appendix B.3.

Verification of the simulation model involved careful tracing of process flow and animation of the model. The material balance recalculation procedure was verified by comparing the results of a simplified model consisting of three tanks to the analytical solution (cf. Eq. 30). It was further verified through checking the overall material balance from inflow into the tank system to its outflow:

$$\int c_{inflow} r_{inflow}\, dt \overset{!}{=} \int c_{outflow} r_{ouflow}\, dt \qquad \text{Eq. 31}$$

where c is byproduct concentration and r is volumetric flow rate.

For validation, the simulation model was run with the input parameter configuration of the current process. The simulation output parameters were then thoroughly compared with the output data acquired for the real process. Means, variations, as well as evolution over time of several parameters were examined and discussed with SMEs. Emphasis was put on validation of the most important key figure, the throughput of the primary feed unit expressed as batches produced per day. The results for the key figure obtained from a simulation run of the current state model are presented in Figure 57. Mean, variance and progression of the figure were in good agreement with the real system, suggesting its validity.

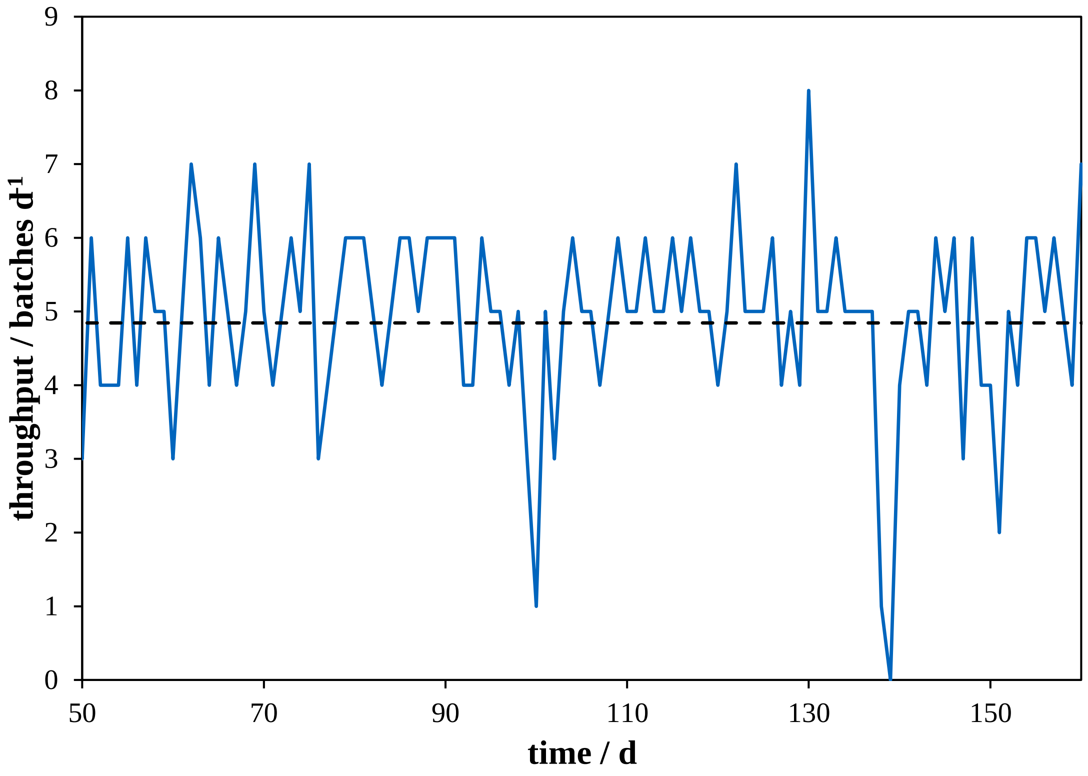


Figure 57: Throughput of the primary feed unit obtained from a simulation run with the current state model of the case study 4 process.

5.4.4 Model experimentation and analysis

When running the simulation model, an initial transient phase was observed, due to the fact that that buffer tanks and storage areas were idle upon initialisation. This entailed an elevated throughput of the primary feed unit during that portion of the run. In order to measure this key figure as well as any further parameters adequately, the initial transient phase was eliminated. This was done with the graphical method developed by Welch (Lavenberg et al. 1981). As a result, the first 50 days of each simulation run were eliminated. The overall run length was set to 170 days, resulting in 120 days being evaluated.

In order to obtain results, which were comparable across different system configurations, a relative error for the mean daily throughput of the primary feed unit of less than ± 0.5 % at a 95 % confidence level was aspired. For this purpose, the simulation was run multiple times for each system configuration in a sequential procedure, in which the relative error was recalculated after each run.

The simulation study was divided into two stages. First, the steady state bottleneck of the main process was examined, neglecting any random variability except for the feed processes. In the second stage, random variability was added and failures in the main process were addressed.

In order to determine the potential of eliminating the steady state bottleneck of the case study process, simulation experiments with the current state model without random failures as well as a model of the feed process only were conducted. Several statistical measures of simulation of both experiments are presented in Table 20. The results led to the conclusion, that the feed process was able to operate at a ~17 % higher rate compared to the main process, setting the quantitative goal for the debottlenecking project. The bottleneck was then sought through sensitivity analysis in a simulation campaign, which included variation of several process parameters. As a result, both the maximum evaporation rate of the evaporation plant, as well as the separation ratio of the reverse osmosis plant (accumulated permeate volume divided by accumulated RO feed volume during a simulation run) was identified as the global bottleneck. Enhancement of either unit resulted in complete bottleneck elimination in the model. Consequently, both parameters were further inspected, in order to determine the minimum effort required for bottlenecking. The results which quantify the required improvements for successful bottleneck elimination are depicted in Figure 58 and Figure 59.

Table 20: Statistical summary for primary feed unit throughput [batches d^{-1}] of case study 4 obtained in simulation experiments without random failures.

System	# runs	Mean	Standard deviation	Confidence interval ±	Relative error ±
Current state; full process	36	5,10	0,075	0,025	0,0049
Current state; feed process only	21	5,95	0,063	0,029	0,0048

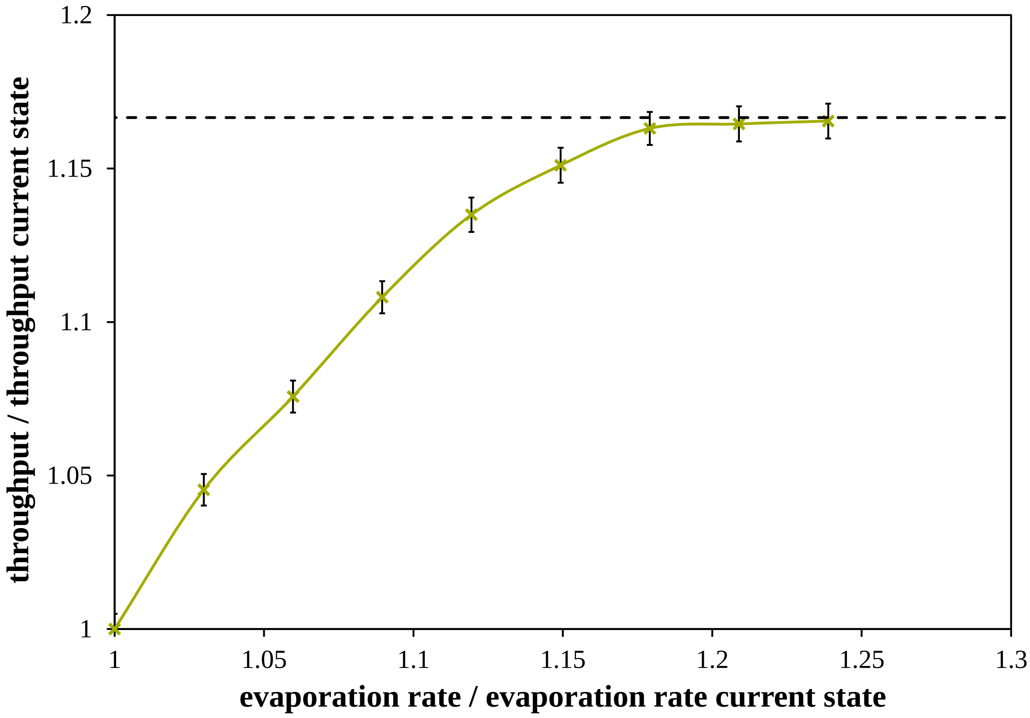


Figure 58: Effect of increasing the evaporation rate on the throughput of the primary feed unit in the simulation model of case study 4 without random failures.

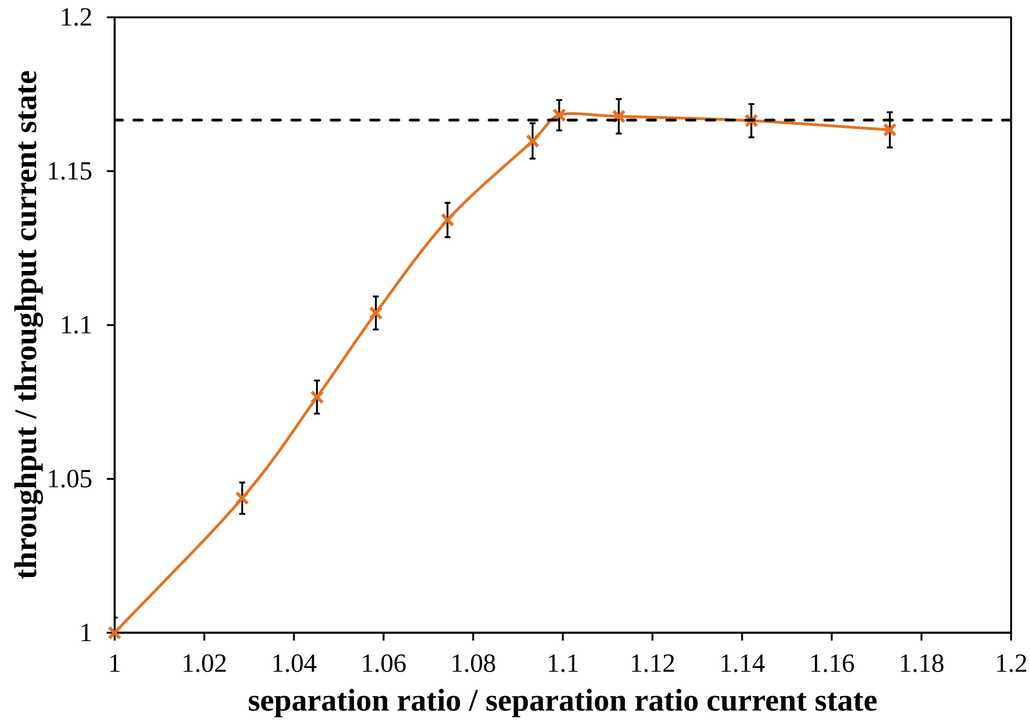


Figure 59: Effect of increasing the RO separation ratio on the throughput of the primary feed unit in the simulation model of case study 4 without random failures.

After the steady state bottleneck was identified and actions for its elimination were quantified, random failures as determined in the conceptual model were added. A simulation campaign, in which stepwise the random failure types were excluded from the model, revealed the impact of each failure type on the primary feed unit throughput. Figure 60 shows the effect of the three major failures of the process as defined in Figure 63 in Appendix B.1. The results indicate that elimination of failure 1 did not significantly improve the process, while the removal of failure 2 or failure 3 had major effects. Thus, technical improvement projects tackling failure 2 and failure 3 could be suggested as effective options for capacity increase of the primary feed unit.

An alternative solution for mitigating the negative effect of random failures was found to be available through optimization of buffer tank utilization, if an increased RO separation ratio or evaporation rate were accomplished. If in that case the RO and evaporation feed rates, which were steered by operator decision (cf. Appendix B.2), were adjusted towards keeping the fill level of their corresponding feed tanks as low as possible, buffers for lowering the effect of random failures on the primary feed unit throughput could be established. The maximum available buffer times for each tank and storage area of the process is shown in Figure 61. Verification of this option with aid of the simulation model proved that significant mitigation of the effect of the more downstream failure types ‘failure 2’ and ‘failure 3’ was possible.

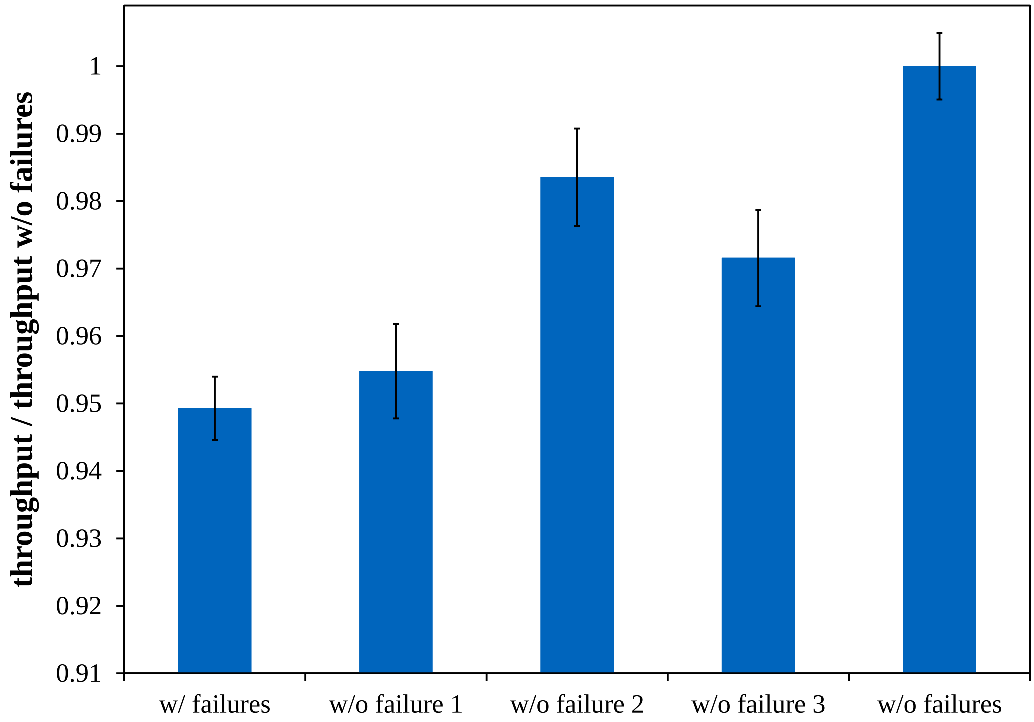


Figure 60: Effect of eliminating random failures as defined in Figure 63 on the throughput of the primary feed unit in the simulation model of case study 4.

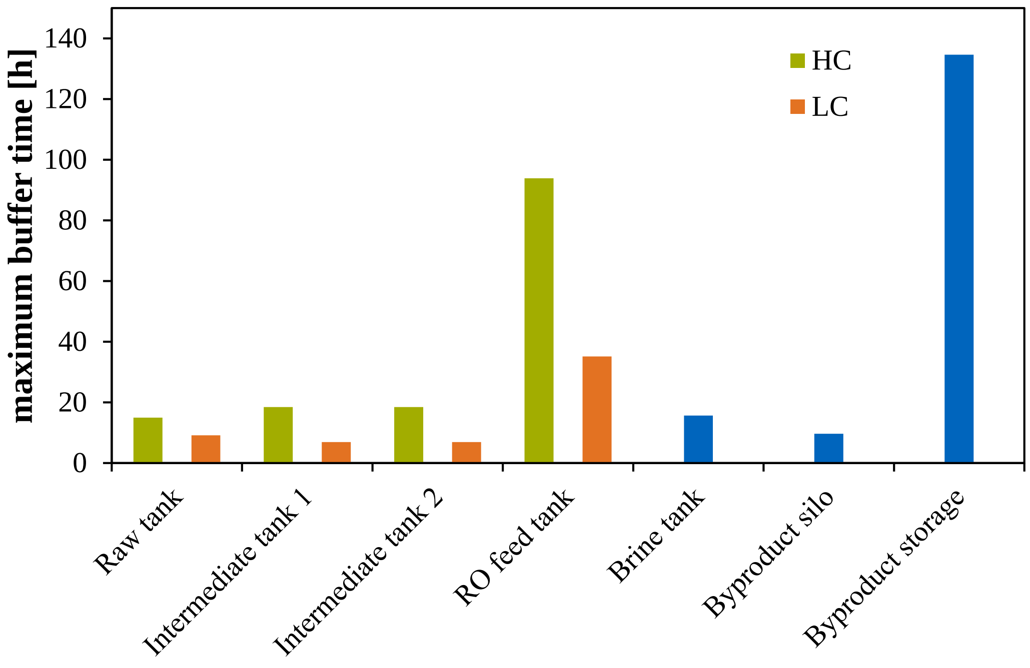


Figure 61: Maximum buffer times available in the process of case study 4.

5.4.5 Discussion

The capability of discrete simulation techniques for modelling, understanding and optimizing processes in the chemical industry has been pointed out by Cope 2010, McGarvey, Dargatz and Dzirbik 2011, Sharda and Bury 2008 and Sharda and Vazquez 2009. However, the majority of the studies reported so far focus on discrete operations and aspects of the chemical industry, such as analytical laboratories, machine failures or dispatch from final product tank farms. Case study 4 covered the application of discrete simulation techniques for modelling an entire, complex chemical production process. As the process comprised both, discretely and continuously operated sections, an enhanced simulation approach was elaborated for adequate modelling. While involving continuous bulk material flow into the model represented no major challenge with the aid of commercially available DES expansions such as ExtendSim® DRS, integrating continuously changing attributes and in particular continuously changing multi-component flow in the discrete simulation model was a rather novel approach. The need to include continuously changing multi-component flow in the model led to the development of a two-stage material balance recalculation procedure with discrete and continuous recalculation points, which assumes plug flow between, and performs backmixing at recalculation points.

The simulation study followed a typical structure, comparable to the approaches outlined by Banks et al. (2009), or Law (2007). Besides the continuous simulation integrated model building, data gathering and input parameter modelling represented a major challenge. In particular, determining and modelling inter- and autocorrelated input parameters inherent to chemical processes represents a complex task (cf. Law 2007 for an introduction to the subject), which provides room for further research. In case study 4 of the thesis, this field was touched with the washing process in the primary feed unit, were autocorrelation was modelled with the aid of Markov chains.

The case study suggests that utilizing enhanced discrete simulation techniques for modelling chemical production processes can be valuable for unravelling optimization potential. Even though chemical processes are in large part operated continuously, discrete events may influence or even govern their performance. The approach presented in this case study provided the opportunity to determine bottlenecks of a transient chemical process. Given the fact that high equipment utilization is key for profitable operation of chemical production plants, such projects which seek to maximize process efficiency are vital for the chemical industry. Simulation models which cover entire production processes including their transient behaviour can potentially be applied as a gainful decision making tool for debottlenecking, extension or even development of new chemical processes.

6. Concluding summary

‘Making more with less’ is an essential factor of success in a globalised economy with emerging scarceness of resources. ‘Making more with less’ is also the core idea behind Lean production systems as developed by the Japanese manufacturing industry, spearheaded by Toyota, which yielded a competitive edge over well-established mass producers. With the prevalence of Lean production in industries beyond Japanese manufacturers over the last decades, Value Stream Mapping has been introduced as a holistic Lean implementation method. VSM has since established itself as an integral tool of Lean or Lean Sigma initiatives which are nowadays launched across the industries. Its success is well-demonstrated by academic research. However, despite its widespread utilization, the method has several shortcomings, in particular in sectors such as the chemical industry, which differ from its original field of application.

The purpose of this thesis was to analyse the applicability and benefit of VSM for optimizing chemical production processes. Additionally, enhancement of the method was aspired in order to eliminate any shortcomings. For this purpose, Discrete Event Simulation has been identified as a valuable tool while elaborating this thesis. Beyond the integration of DES into VSM, its deployment DES for optimization of chemical production processes was further explored.

The experimental section of the thesis is structured into four case studies, which cover optimization projects for chemical production processes. Case study 1 and case study 2 focus on the application of VSM to chemical processes as well as adaption and enhancement of the method. In case study 3 and case study 4 the application of DES as a general tool for chemical process optimization is analysed and refined. With the exception of case study 3, which is based on a model process, all case studies cover real world production processes in Clariant.

The shortcomings of VSM when applying the method to chemical processes were found to be of manifold nature. One major drawback of VSM is closely related to one of its major strengths, the straightforwardness of the “paper and pencil” method, which allows direct involvement of all stakeholders along the value stream in the optimization procedure. In complex production environments with non-linear flow, which are predominantly found in chemical processes, the material balance may not be captured adequately when “walking the process”. VSM also lacks the ability to involve variability and process dynamics. A Value Stream Map only provides a snapshot of the process which may, in case of transient behaviour, lead to false conclusions and ultimately an iterative implementation procedure of the proposed future state. Another shortcoming of VSM is related to the future state guidelines as propagated by the method. Batch size reduction and an increased frequency of changeovers may lead to inventory reduction, flexible Just In Time production and One Piece Flow. At the same time however, it may entail an increase of major cost components such as raw material or energy consumption.

For the purpose of eliminating these shortcomings, a DES enhanced VSM procedure was elaborated. While the original VSM procedure up to including the design of the future state map remains untouched in order to preserve the strengths of the method, a DES feasibility and trade-off analysis is incorporated into the approach after completion of the future state map. With additional data gathering to cover the complexity as well as the dynamics of the process, a DES model is composed, which is capable of answering the two questions:

- Is the proposed future state able to meet the customer demand?
- Does the proposed future state result in the optimal process when all cost components are considered?

Case study 1 analyses the benefit of the VSM when applying it to chemical processes and elaborates its shortcomings which led to development of the DES enhanced method. In case study 2, DES enhanced VSM is applied to a chemical production process, proving the capability to eliminate the above outlined shortcomings.

Despite the demonstration of its applicability, the DES enhanced VSM procedure provides room for further research. More industrial case studies are required to verify the usefulness and to increase the confidence in the approach. In addition, modelling of the cost components for conducting the feasibility analysis remains challenging. VSM may affect producer objectives in delay as well as market objectives, which can both not be included in an objective function straightforwardly. Here, concepts like Pareto efficiency may be worth exploring.

A weak point of DES for modelling chemical processes is addressed in case study 3 and case study 4. DES is tailored to modelling the transient flow of discrete items. However, in chemical production, predominantly bulk material is processed. This explains the rather scarce deployment of the simulation technique in the chemical industry. Coupling of DES with Discrete Rate Simulation as well as continuous simulation eliminates this weak point, which is demonstrated in this thesis. The approach is capable of modelling bulk material flow as well as continuously changing attributes, while preserving the ability to involve variability.

In case study 3, the mixed simulation approach is applied to a cost optimization project involving several cost components, which could as well be under consideration in a VSM project. In case study 4, debottlenecking of a complex multi-stage process is approached with a mixed DES, DRS and continuous simulation model. Both case studies reveal that coupling DES and DRS is straightforwardly possible. Adding continuous simulation to the approach, however, leads to significant increase of complexity. When a continuously changing attribute needs to be included in the model, two general cases can be identified – either the attribute depends on the flow media composition or not. In case it does not depend on the flow media composition, but for instance on the variation of pressure or temperature or merely the accumulated volume of flow media, it is sufficient to deploy continuous recalculation only in the model section involving the continuously changing attribute. If it does depend on flow media composition on the other hand, tracing of the material balance with continuous recalculation is required between the root cause of the composition variation and the continuously changing attribute.

Case study 3 and case study 4 suggest that combination of all three simulation types provides a promising toolset for adequately modelling complex transient chemical processes. Room for additional research however, is found for adequate simulation input parameter modelling of chemical processes, in particular if correlation between parameters or autocorrelation of individual parameters is identified. Furthermore, it is worth exploring a standard procedure for determining the minimum required step size for continuous recalculation in order to reduce the CPU effort for executing the simulation model, which is significantly increased when adding continuous simulation to DES and/or DRS.

7. Abschließende Zusammenfassung

In einer globalisierten Wirtschaftswelt mit sinkender Ressourcenverfügbarkeit ist Effizienzsteigerung von Produktionsprozessen ein entscheidender Erfolgsfaktor. Effizienzsteigerung ist auch das Hauptziel der in der japanischen Industrie vor allem durch Toyota entwickelten Lean-Produktionssysteme, welche einen entscheidenden Wettbewerbsvorteil gegenüber den weltweit etablierten Massenproduktionssystemen boten. Mit der Verbreitung von Lean-Produktionssystemen auch außerhalb von Japan, wurde die Wertstromanalyse als ganzheitliche Lean-Implementierungsmethode entwickelt. Seit ihrer Einführung hat sich die Wertstromanalyse als Zentrales Werkzeug in Lean und Lean Sigma Initiativen etabliert, welche heutzutage in verschiedensten Industriezweigen Einzug halten. Die Effektivität von Wertstromanalysen wurde bereits durch zahlreiche wissenschaftliche Veröffentlichungen belegt. Allerdings offenbart die Methode trotz ihrer weiten Verbreitung auch einige Schwachstellen, vor allem bei deren Anwendung in Sektoren, die sich stärker vom ursprünglichen Anwendungsgebiet in der mechanischen Fertigung unterscheiden. Dies ist beispielsweise in der chemischen Industrie der Fall.

Das Ziel der vorliegenden Arbeit war es, die Anwendbarkeit sowie die Effektivität von Wertstromanalysen in der chemischen Industrie zu analysieren. Zudem sollte die Methode weiterentwickelt werden, um deren Schwachstellen bei der Anwendung auf chemische Prozesse zu beseitigen. Zu diesem Zweck konnte im Laufe der Arbeit Discrete Event Simulation als nützliches Werkzeug identifiziert werden. Über die Einbindung der Simulationstechnik in Wertstromanalysen hinaus, wurde der Einsatz von DES als alleinstehendes Tool zur Optimierung chemischer Prozesse getestet.

Der Experimentalteil der vorliegenden Arbeit ist in vier Fallstudien gegliedert, welche Projekte zur Optimierung chemischer Produktionsprozesse beschreiben. Während Studie 1 und Studie 2 die Anwendbarkeit und Weiterentwicklung der Wertstromanalyse für chemische Prozesse behandeln, wird in Studie 3 und Studie 4 DES als alleinstehendes Werkzeug zur Optimierung chemischer Prozesse genutzt und weiterentwickelt. Mit Ausnahme von Studie 3, welche einen Modellprozess beschreibt, wurden die Studien mit realen Produktionsprozessen bei Clariant durchgeführt.

Die Schwachstellen der Wertstromanalyse bei deren Anwendung in der chemischen Industrie sind vielfältiger Natur. Ein Nachteil der Methode steht im direkten

Zusammenhang mit einer ihrer Stärken, der Einfachheit, welche die direkte Einbindung aller Beteiligten entlang eines Wertstroms zulässt. In komplexen Produktionsprozessen mit nicht-linearem Materialfluss, welche häufig in der chemischen Industrie zu finden sind, lässt sich dieser nicht exakt erfassen, während man dessen Verlauf physisch folgt. Darüber hinaus bietet die Wertstromanalyse keine Möglichkeit, die Variabilität und Dynamik von Prozessen abzubilden. Die Wertstromanalyse basiert auf einer Momentaufnahme des Prozesses, welche im Fall von stärkeren Prozessschwankungen zu falschen Schlussfolgerungen und einem iterativen Implementierungsprozedere führen kann. Eine weitere Schwachstelle ist in den von der Methode vorgegebenen Optimierungs-Guidelines zu finden. Die Reduktion von Chargengrößen und Erhöhung der Produktwechselfrequenz führen zu einer Reduktion der Bestände und flexibler Just-in-Time Produktion. Allerdings können sie auch zu einer Erhöhung verschiedenster Kostenkomponenten, wie beispielsweise eingesetzten Rohstoffen oder Energieverbräuchen führen.

Um die Schwachstellen zu beseitigen, wurde eine mit DES erweiterte Wertstromanalysenmethode erarbeitet. Hierbei bleibt das ursprüngliche Prozedere bis zur Entwicklung des optimierten Prozesses zunächst unberührt, um die Stärken der Methode zu wahren. Darauffolgend wird vor der Implementierung des Optimierungsvorschlags eine Machbarkeits- und Zielkonfliktanalyse mithilfe von DES durchgeführt. Auf Basis der Wertstromanalyse, sowie zusätzlicher Aufnahme von Daten zur Prozessvariabilität und -dynamik wird ein DES Modell erstellt, welches in der Lage ist, die folgenden beiden Fragen zu beantworten:

- Lässt sich mit dem Vorschlag zur Prozessoptimierung der Kundenbedarf decken?
- Führt der Optimierungsvorschlag tatsächlich zu einem unter Berücksichtigung aller Kostenkomponenten optimalen Prozess?

In Fallstudie 1 wird der Nutzen von Wertstromanalysen bei deren Anwendung on der chemischen Industrie analysiert und die Schwachstellen aufgedeckt, welche zur Entwicklung der mit DES erweiterten Methode führten. In Fallstudie 2 wird eine mit DES erweiterte Wertstromanalyse anhand eines chemischen Prozesses durchgeführt, und damit das Potential der Methode belegt, die Schwachstellen zu beseitigen.

Trotz der Erkenntnisse aus den beiden Fallstudien bietet die mit DES erweiterte Wertstromanalyse weitere Forschungs- und Entwicklungsmöglichkeiten. Weitere

Studien sind vonnöten, um die Anwendbarkeit der Methode, sowie deren Flexibilität zu verifizieren. Zudem stellt die Modellierung der Kostenkomponenten für die Zielkonfliktanalyse eine Herausforderung dar. Wertstromanalysen können verzögerte Auswirkung auf Betriebsziele oder Marktziele haben, welche nicht direkt in einer Zielfunktion berücksichtigt werden können. Hier könnten Konzepte wie beispielsweise die Pareto-Effizienz Abhilfe schaffen.

In Fallstudie 3 und 4 wird eine Schwachstelle von DES bei deren Anwendung zur Modellierung chemischer Prozesse aufgedeckt. DES bietet primär die Möglichkeit, instationären Fluss diskreter Elemente zu modellieren. In chemischen Prozessen werden allerdings größtenteils kontinuierliche Medien verarbeitet. Dies erklärt auch die relative spärliche Anwendung von DES in der chemischen Industrie. In der vorliegenden Arbeit konnte gezeigt werden, dass die Einbindung von Discrete Rate Simulation und kontinuierlichen Simulationstechniken in DES-Modelle die Abbildung komplexer instationärer chemischer Prozesse ermöglicht.

In Fallstudie 3 wird der Simulationsansatz genutzt, um eine Produktionskostenoptimierung eines chemischen Prozesses mit mehreren Kostenkomponenten durchzuführen. In Fallstudie 4wird eine Kapazitätserhöhung eines komplexen mehrstufigen Prozesses mithilfe von DES, DRS und kontinuierlichen Simulationstechniken angestrebt. Beide Fallstudien zeigen, dass eine Verbindung von DES und DRS sehr leicht möglich ist. Die Einbindung kontinuierlicher Simulationstechniken allerdings führt zu einer signifikanten Steigerung der Komplexität. Kontinuierlich veränderliche Eigenschaften eines chemischen Prozesses lassen sich aus simulationstechnischer Sicht in zwei grundlegende Fälle einteilen – entweder hängt die Eigenschaft von der Zusammensetzung des Flussmediums ab oder nicht. Wenn sie nicht von der Zusammensetzung des Flussmediums abhängt, sondern beispielsweise von Druck, Temperatur oder der akkumulierter Menge an Flussmedium, reicht es aus, nur den Prozessabschnitt mit der kontinuierlich veränderlichen Eigenschaft mit kontinuierlichen Simulationstechniken zu modellieren. Wenn sie von der Zusammensetzung des Flussmediums abhängt, muss allerdings die Stoffbilanz mittels kontinuierlicher Simulationstechniken zwischen dem Ursprung der Variabilität der Zusammensetzung und dem Abschnitt mit der kontinuierlich veränderlichen Eigenschaft modelliert werden.

Fallstudie 3 und 4 zeigen, dass die Kombination der drei Simulationstechniken ein leistungsfähiges Werkzeug bietet, welches in der Lage ist, komplexe instationäre chemische Prozesse zu modellieren. Weiterer Forschungs- und Entwicklungsbedarf besteht allerdings bei der Modellierung der Variabilität von Prozessparametern als Input für die Simulationsmodelle. Dies ist besonders anspruchsvoll, wenn unterschiedliche Parameter miteinander korrelieren oder im Fall von Autokorrelation einzelner Parameter. Zudem wäre es hilfreich, ein Standardverfahren für die minimal erforderliche Schrittgröße zwischen den kontinuierlichen Neuberechnungen der Simulationsmodelle zu entwickeln, um den Rechenaufwand während der Simulation zu minimieren, welcher erheblich ansteigt, wenn man kontinuierliche Simulationstechniken in ein DES und/oder DRS Modell einbindet.

Appendix A: Supplementary data for case study 3

A.1 Process flow diagram

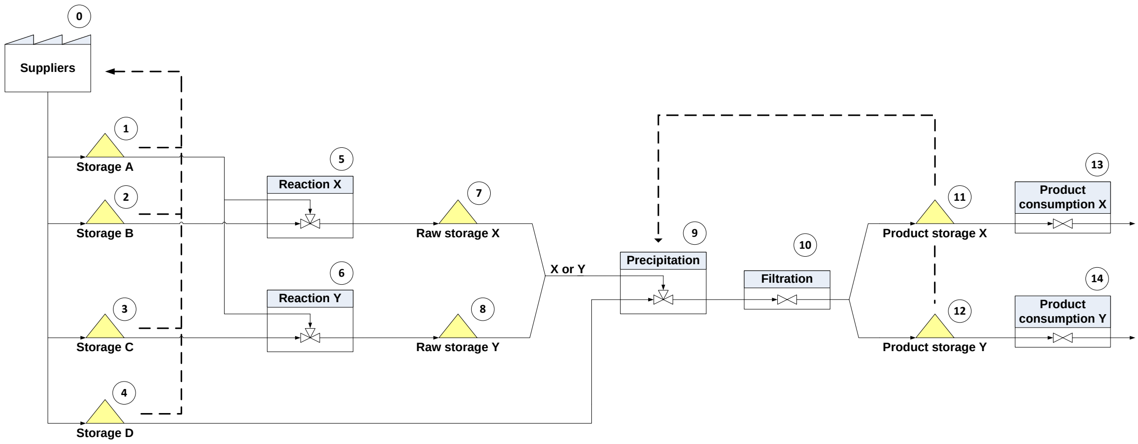


Figure 62: Process flow diagram for case study 3 simulation model.

A.2 Material balance

Product X: $1\,A + 1\,B + 1D \;\rightarrow 1X$

Product Y: $1\,A + 1\,C + 1D \;\rightarrow 1Y$

A.3 Process

0: Suppliers:

- Each raw material can be supplied in batches of 20, 40, 60 or 80 units
- Delivery time: 5 days (A), 10 days (A), 8 days (C), 5 days (D)
- Raw material costs: 3000 € /unit A, 5000 € /unit B, 2000 € /unit C, 1500 € /unit D
- Additional expenses: 1000 €/delivery

1, 2, 3, 4: Storage A, B, C, D:

- Capacity: 230 units of each raw material
- Orders: Orders can be placed at fill levels between 10 and 150 units for each raw material

5, 6: Reaction X, Y:

- 1A + 1B (product X) and 1A + 1C (product Y) react in a batch process
- Batch time: 8 – 16 h (product X), 7 – 20 h (product Y)

7, 8: Raw storage X, Y:

- Capacity: 200 m^3 for each material
- Specific volume: 10m^3/unit raw X, 10 m^3/unit raw Y
- Storage tanks can be arbitrarily changed with tanks of product storage X, Y

9: Precipitation:

- 1 raw X or 1 raw Y is precipitated with 1D in a batch process
- Specific volume: 10m^3/unit (X and Y)
- Batch time: 1.5 – 4.5 h
- Changeover time: 16 h
- Changeover costs: 1000 €

10: Filtration:

- Filtration under constant pressure
- Solid content of filtration feed is constant
- Filtrate is product, filter cake is waste
- Filter press is cleaned when volumetric flow rates fall below a certain level between 1 -18 m^3/h, depending on the design parameter setting
- Cleaning time: 5 h
- Volumetric flow rate (Q) calculates as:

$$Q = \frac{1}{a_1 \cdot V + a_0} \qquad \text{Eq. 32}$$

$$a_0 = \frac{\eta \cdot \beta}{A_F \cdot \Delta p_f} \qquad \text{Eq. 33}$$

$$a_1 = \frac{\eta \cdot \alpha \cdot k_k}{2 \cdot {A_F}^2 \cdot \Delta p_f} \qquad \text{Eq. 34}$$

where V is volume of filtrate, η is dynamic viscosity, β is resistance of the filter medium, A_F is filter area, Δp_f is differential pressure over filter cake and filter medium, α is specific resistance of the filter cake and k_k is the ratio of accumulated filter cake volume to accumulated volume of filtrate.

– Filtration parameters: a_0 = 166.67 s m^{-6}, a_1 = 16.667 s m^{-3}
– Cleaning costs: 200 €
– Operating costs: 70 €/h

11, 12: Product storage X, Y:

– Capacity: 100 m³ (X), 300 m³ (Y)
– Specific volume: 10 m³/unit X, 10 m³/unit Y
– Storage tanks can be arbitrarily changed with tanks of raw storage X, Y
– Production orders can be sent to precipitation unit at fill levels between 10 and 60 %
– Production stop orders can be sent to precipitation unit at fill levels between 50 and 100 %

13, 14: Product consumption X, Y:

– Product is consumed by downstream processes at 0.75 – 1.5 units/day (X) and 1.1 – 2.4 units/day (Y)
– Idle time results in revenue loss of 5000 €/unit X and 3500 €/unit Y

A.4 Variability

– Reaction time 5: Triangular distribution (most likely: 12, min: 8, max: 16) [h/unit]
– Reaction time 6: Triangular distribution (most likely: 10, min: 7, max: 20) [h/unit]
– Precipitation time 9: Triangular distribution (most likely: 3, min: 1.5, max: 4.5) [h/unit]
– Consumption time 13: Triangular distribution (most likely: 24, min: 16, max: 32) [h/unit]
– Consumption time 14: Triangular distribution (most likely: 16, min: 10, max: 22) [h/unit]

A.5 Objective function

$$
\begin{aligned}
min\Bigg\{\Bigg(&\int_{0}^{4000h}(A\ delivered - X\ consumed - Y\ consumed)dt \cdot 3000\frac{€}{unit} \\
&+ \int_{0}^{4000h}(B\ delivered - X\ consumed)dt \cdot 5000\frac{€}{unit} \\
&+ \int_{0}^{4000h}(C\ delivered - Y\ consumed)dt \cdot 2000\frac{€}{unit} \\
&+ \int_{0}^{4000h}(D\ delivered - X\ consumed - Y\ consumed)dt \\
&\cdot 1500\frac{€}{unit}\Bigg) \cdot 10\% \cdot \frac{4000h}{8760h} \\
&+ (\#deliveries\ A + \#deliveries\ B + \#deliveries\ C \\
&+ \#deliveries\ D) \cdot 1000\frac{€}{delivery} + idle\ time\ consumption\ X \\
&\cdot \frac{5000\frac{€}{unit}}{24\frac{h}{unit}} + idle\ time\ consumption\ Y \cdot \frac{3500\frac{€}{unit}}{16\frac{h}{unit}} \\
&+ filter\ press\ operation\ time \cdot 70\frac{€}{h} \\
&+ \#filter\ press\ cleaning\ cycles \cdot 200\frac{€}{cycle} + \#changeovers \\
&\cdot 1000\frac{€}{changeover}\Bigg\}
\end{aligned}
\qquad \text{Eq. 35}
$$

Appendix B: Supplementary data for case study 4

B.1 Process flow diagram

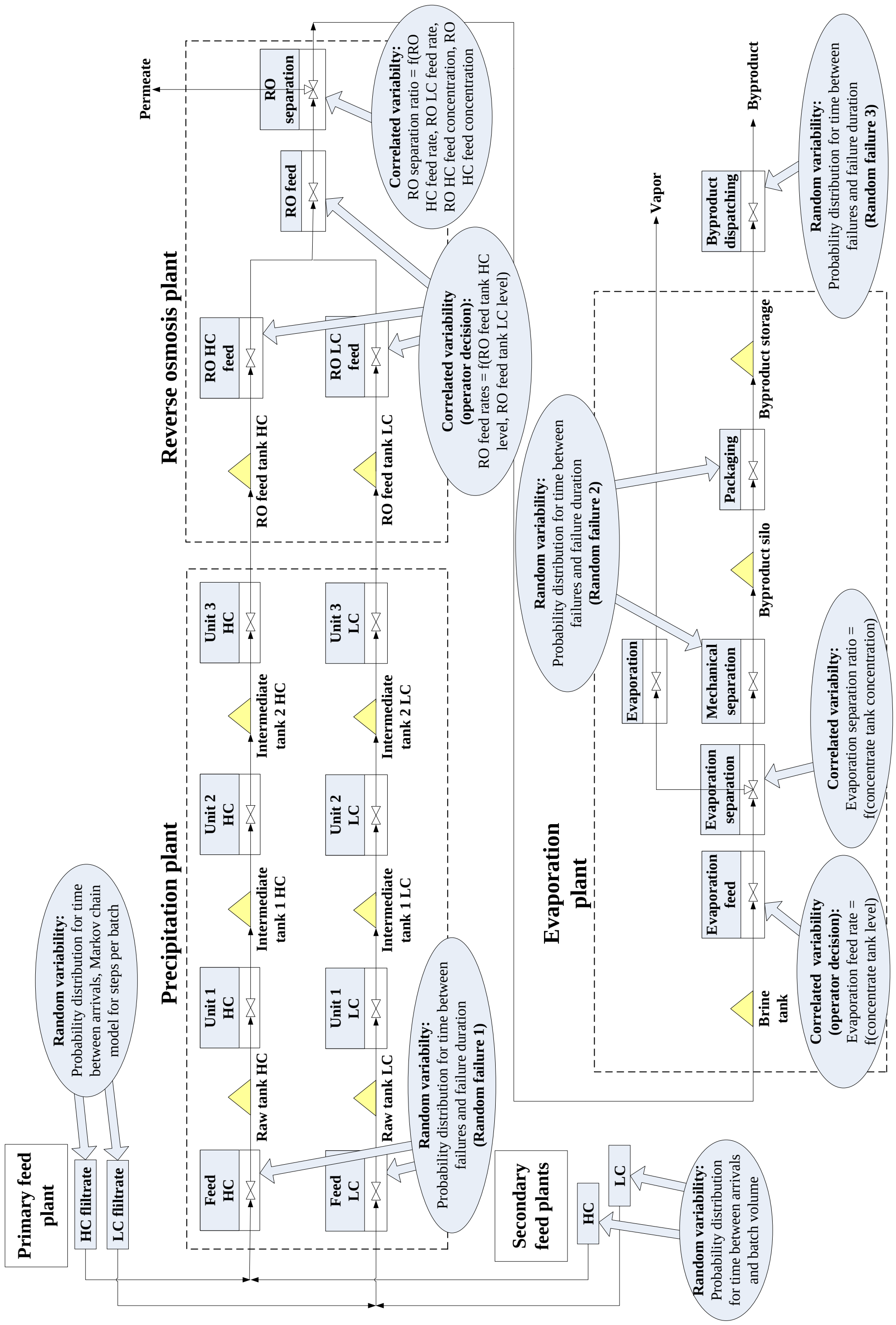


Figure 63: Process flow diagram for case study 4 simulation model.

B.2 Process and variability

Primary feed unit:

Table 21: Process data and variability of primary feed unit in case study 4.

Step	Av. duration [h]	Duration distribution	Feed volume [m³]	Feed concentration [kg m^{-3}]	Line
Changeover	1.88	Gamma (α = 6.84511; β = 0.275167)	-	-	-
Mother liquor HC	0.33	-	5.1	110.5	HC
Mother liquor LC	0.17	-	5.1	49.0	LC
1st wash	0.67	-	18.3	29.5	LC
2nd & 3rd wash	0.5	-	-	-	-
4th wash	0.5	-	5.2	0	LC
5th wash	0.5	-	7.5	0	LC

Table 22: Markov chain transition matrix with probabilities for the requirement of the fourth washing step in the primary feed unit in case study 4.

Fourth washing step requirement in the previous three batches			Fourth washing step required	
antepenultimate	penultimate	previous	yes	no
no	no	no	0.289	0.711
no	no	yes	0.574	0.426
no	yes	no	0.488	0.512
yes	no	no	0.352	0.648
yes	no	yes	0.625	0.375
yes	yes	no	0.459	0.541
no	yes	yes	0.770	0.230
yes	yes	yes	0.803	0.197

Table 23: Markov chain transition matrix with probabilities for the requirement of the fifth washing step in the primary feed unit in case study 4. Probabilities for the fifth washing step apply only in case the fourth washing step was required.

Number of washing steps required in the previous two batches		Fifth washing step required	
penultimate	previous	yes	no
four	four	0.556	0.444
four	five	0.590	0.410
five	four	0.487	0.513
five	five	0.799	0.201
three	five	0.714	0.286
three	four	0.577	0.423
five	three	0.654	0.346
four	three	0.273	0.727
three	three	0.537	0.463

Secondary feed units:

Table 24: Process data and variability of secondary feed units in case study 4.

Unit	Av. time between arrivals [d]	Time between arrivals distribution	Av. volume [m³]	Volume distribution	Con-centration [kg m^{-3}]	Volumetric flow rate [m³ h^{-1}]	Line
HC unit 1	3.9122	Gamma (α = 2.15059; β = 1.57688)	15.7	Triangular (min = 10.7; max = 20.7)	160	4.01	HC
HC unit 2	2	Triangular (min = 1.3; max = 2.7)	6	Triangular (min = 10; max = 25)	70	8.75	HC
LC unit 1	1.8398	Johnson S_U (λ= 6.458; γ = -0.162; δ = 0.5744; location = 30.06)	17.5	-	30	3.26	LC
LC unit 2	2	Triangular (min = 1.3; max = 2.7)	15.5	Triangular (min = 10.5; max = 20.5)	30	7.75	LC

Precipitation plant:

– Inflow to raw tank HC/LC:

Feed from only one feed unit at a time possible; feeding only possible if available volume in raw tank < feed volume; time between failures: exponential distribution (mean = 240 h; location = 1 h); failure duration: exponential distribution (mean = 3 h; location = 1 h)

- Raw tank HC/LC:
  Volume = 43 m^3 (HC) and 70 m^3 (LC)
- Unit 1 HC/LC:
  Volumetric flow rate = 15 $m^3\ h^{-1}$; unit is only operating when inflow to raw tank is not operating
- Intermediate tank 1 HC/LC:
  Volume = 53 m^3 (each line)
- Unit 2 HC/LC:
  Volumetric flow rate = 12 $m^3\ h^{-1}$
- Intermediate tank 2 HC/LC:
  Volume = 53 m^3 (each line)
- Unit 3 HC/LC:
  Volumetric flow rate = 11 $m^3\ h^{-1}$; unit is disabled when volume of RO feed tank reaches 250 m^3 and is restarted when volume of RO feed tank falls below 200 m^3

Reverse osmosis plant:

- RO feed tank HC/LC:
  Volume = 270 m^3 (each line)
- RO feed HC/LC:
  Maximum volumetric flow rate = 5 $m^3\ h^{-1}$ (HC) and 10 $m^3\ h^{-1}$ (LC); actual volumetric flow rates depend on fill volumes of RO feed tanks and brine tank (see Table 25) and are to be modelled with the aid of volume indicators (see Figure 64)

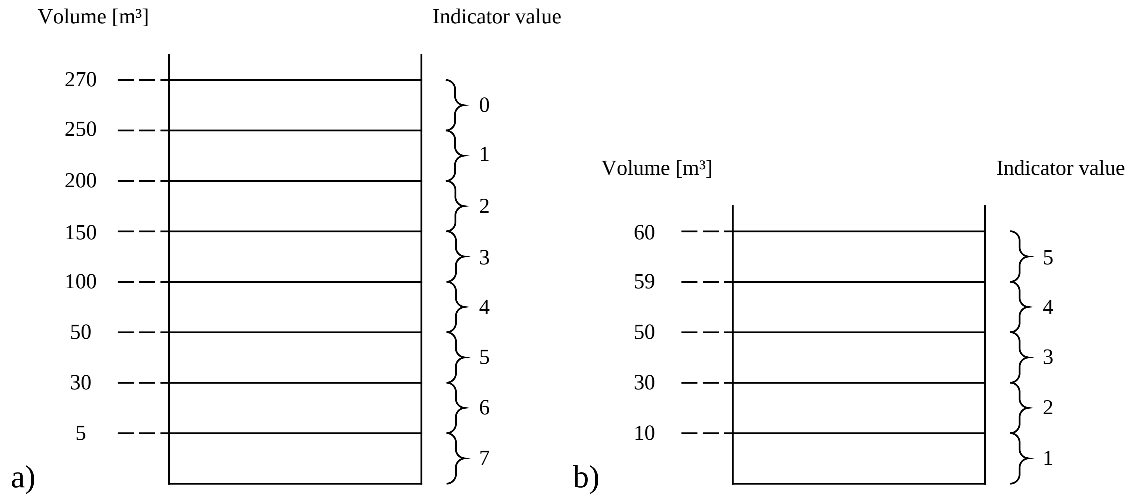


Figure 64: Visualisation of volume indicators in RO feed tank HC and LC (a) and brine tank (b) of case study 4.

Table 25: Effect of fill volumes of RO feed tanks on RO feed rates in case study 4.

Indicator values of RO HC and LC feed tanks or brine tank	Result on RO feed
HC or LC ≤ 4	Start feeding
HC = 7 and LC ≥ 5	Stop feeding
HC ≥ 5 and LC = 7	Stop feeding
Brine ≤ 3	Start feeding
Brine = 5	Stop feeding
HC ≥ 5 and LC ≥ 5	HC feed rate + LC feed rate = 8 m³ h^{-1}
HC ≤ 2 and LC ≤ 2	HC feed rate + LC feed rate = 14 m³ h^{-1}
HC – LC ≥ 2	Ratio of feed rate HC / feed rate LC = 2 / 8
HC – LC ≤ 2	Ratio of feed rate HC / feed rate LC = 2 / 3
HC – LC = 2	Ratio of feed rate HC / feed rate LC = 3 / 8

– RO separation ratio:
  To be modelled with the aid of multiple linear regression; function of feed volumetric flow rate, HC feed to overall feed volumetric flow rate ratio and byproduct concentration of HC and LC feed

$$\frac{\dot{V}_{permeate}}{\dot{V}_{feed}} = 0.88376 + \frac{\dot{V}_{HC\,feed}}{\dot{V}_{feed}} \cdot (-0.28214) + c_{HC\,feed} \cdot (-0.00141) + c_{LC\,feed} \cdot (-0.00065) \qquad \text{Eq. 36}$$

where $\dot{V}$ is volumetric flow rate in $m^3\ h^{-1}$ and c is byproduct concentration in kg m^{-3}.

Evaporation plant:

- Brine tank:
  Volume = 60 m³
- Evaporation feed:
  Volumetric flow rate changes to 3.35 $m^3\ h^{-1}$ if volume indicator of brine tank ≥ 4; volumetric flow rate changes to 2.5 $m^3\ h^{-1}$ if volume indicator of brine tank ≤ 2
- Evaporation separation:
  Byproduct is fully separated from solvent; conversion from volumetric flow rate to mass flow in order to determine separation ratio

$$\rho = 0.63965 \cdot c + 998.18933 \qquad \text{Eq. 37}$$

$$\dot{m} = \dot{V} \cdot \rho \qquad \text{Eq. 38}$$

where ρ is density in in kg m^{-3}, c is byproduct concentration in kg m^{-3}, $\dot{m}$ is mass flow in kg h^{-1} and $\dot{V}$ is volumetric flow rate in $m^3\ h^{-1}$.

- Mechanical separation:
  Maximum salt mass flow 2,500 kg h^{-1}; time between failures: exponential distribution (mean = 348 h; location = 1 h); failure duration: exponential distribution (mean = 8.85185 h; location = 1 h); failures effect shutdown of evaporation plant
- Byproduct silo:
  Maximum fill level = 5,000 kg
- Packaging:

Packaging rate = 5,000 kg h^{-1}; Discretisation = 1,000 kg $pack^{-1}$; time between failures: exponential distribution (mean = 567 h; location = 1 h); failure duration: exponential distribution (mean = 15.6875 h; location = 3 h)

- Byproduct storage:
  Maximum fill level = 70,000 kg

Byproduct dispatching:

Time between truck arrivals = 72 h; truck capacity = 50,000 kg; Probability of a truck being delayed = 20 %; delay duration = 145 h

B.3 Material balance recalculation algorithm for simulation model

- The algorithm for material balance recalculation as elaborated below is applied in identical form for both, the HC and LC line
- At recalculation points, byproduct concentrations, volumes and volumetric flow rates are represented by vectors (see Figure 65 for notation details and Table 26 for vector definition)
- For calculation of byproduct concentration, a volume transition matrix '$V_{M, i, j}$' as introduced in Table 27 is utilised.
- Actual current volumetric flow rates are sent from the DES/DRS model to global array 'GAr', which is equal in dimension and notation to the vector 'r'
- In between recalculation steps, byproduct concentrations, volumes and volumetric flow rates from the previous recalculation step are stored in the global arrays 'GAc_{old}', GAV_{old}' and GAr_{old}', which are equal in dimension and notation to the vectors 'c_{old}', V_{old}' and 'r'
- A flow chart for the material balance recalculation algorithm is provided in Figure 66

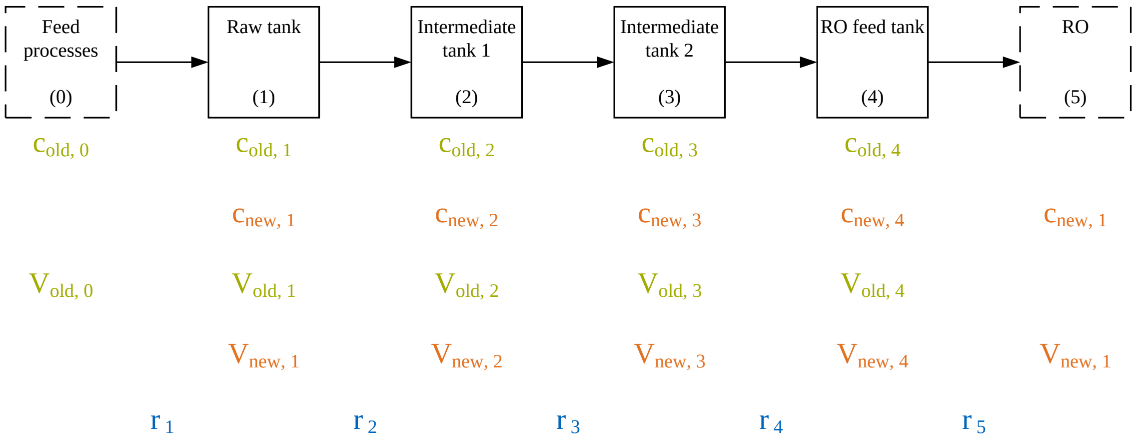


Figure 65: Byproduct concentration (c), volume (V) and volumetic flow rate (r) notation for material balance recalculation algorithm of case study 4 simulation model. The subscript 'old' refers to the previous recalculation point, the subscript 'new' to the current recalculation point.

Table 26: Byproduct concentration (c), volume (V) and volumetric flow rate (r) vectors for material balance recalculation algorithm of case study 4 simulation model. The subscript 'old' refers to the previous recalculation point, the subscript 'new' to the current recalculation point.

c_{old}	c_{new}	V_{old}	V_{new}	r
$\begin{pmatrix} c_{old,4} \\ c_{old,3} \\ c_{old,2} \\ c_{old,1} \\ c_{old,0} \end{pmatrix}$	$\begin{pmatrix} c_{new,5} \\ c_{new,4} \\ c_{new,3} \\ c_{new,2} \\ c_{new,1} \end{pmatrix}$	$\begin{pmatrix} V_{old,4} \\ V_{old,3} \\ V_{old,2} \\ V_{old,1} \\ V_{old,0} \end{pmatrix}$	$\begin{pmatrix} V_{new,5} \\ V_{new,4} \\ V_{new,3} \\ V_{new,2} \\ V_{new,1} \end{pmatrix}$	$\begin{pmatrix} r_5 \\ r_4 \\ r_2 \\ r_2 \\ r_1 \end{pmatrix}$

Table 27: Volume transition matrix $V_{M, i, j}$ for material balance recalculation algorithm of case study 4 simulation model.

	j = 1-5
i = 0-4	$\begin{pmatrix} i = 4, j = 5 & \cdots & i = 4, j = 1 \\ \vdots & \ddots & \vdots \\ i = 0, j = 5 & \cdots & i = 0, j = 1 \end{pmatrix}$

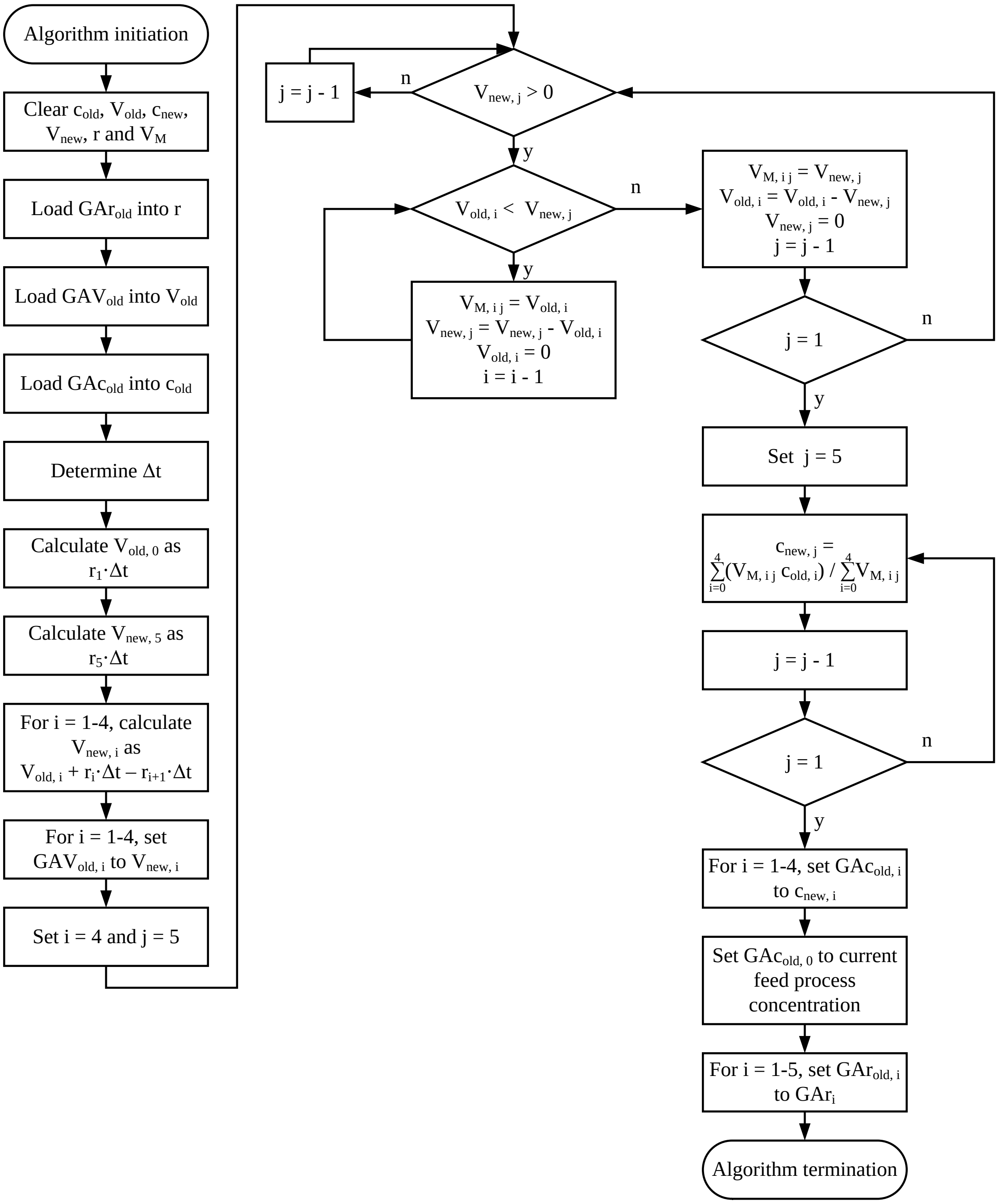


Figure 66: Material balance recalculation algorithm of case study 4 simulation model. The algorithm is initiated with volumetric flow rate changes within GAr (discrete event recalculation) and after time increments $\Delta t = 0.1$ h (continuous recalculation).

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Education

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10/2008 – 2/2009	**University of California Berkeley** – Research project: *"Mechanistic Studies of Ethanol Oxidation on Alumina Supported Vanadium Oxide Catalysts"* in the Alexis Bell Research Group
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Internships

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08/2007 – 01/2008	**Süd-Chemie AG** – Working student at the Environment, Health, Safety & Quality department at the Moosburg site
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