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SIMULATION AND OPTIMIZATION-BASED PLANNING OF THE USE OF TANK CONTAINERS IN THE PRODUCTION OF SPECIALTY CHEMICALS

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ABSTRACT

Changing market conditions in the chemical industry are leading to an increased demand for fast and individually engineered chemicals. This results in a decline in mass production towards producing small, demand-driven quantities. A combination of changing demand and the need for short-term adjustments requires flexible production planning and logistics. To ensure logistics flexibility, primarily manual processes are used. However, this comes with the risk of direct contact between humans and chemicals. One way to avoid this contact and enable sufficient flexibility is to use tank containers directly connected to the production plants. This paper aims to develop a framework that combines simulation and optimization for planning the use of tank containers. Based on this framework, tank container storage materials will be selected using optimization. Furthermore, simulation helps to evaluate the influences of the selection on the logistics system. Here, the focus is on the management of general cargo containers.

1 INTRODUCTION

Global sales in the chemical industry have quadrupled over the last twenty years, because of the growth of the demand for basic chemicals (European Chemical Industry Council 2024). European chemical producers benefit only slightly from this growth. This is due to the low complexity of producing crude oil-related basic chemicals, such as chlorine or hydrogen, which enables emerging countries with limited knowledge to produce them. Additionally, the geographical proximity of the emerging countries to raw material sources is a crucial factor in combination with low wages and resulting low production costs for these countries (Baerns et al. 2014). As a result, many high-wage countries, such as Germany, focus on producing profitable and complex specialty chemicals and avoid exporting basic chemicals by investing in local production in emerging countries. These specialty chemicals have a shorter product life cycle and are produced in smaller, demand-driven quantities than basic chemicals. Price and availability are not the primary considerations. These characteristics lead to volatile sales markets with high product differentiation and smaller production volumes. The resulting change in customer demand behavior from basic chemicals to specialty chemicals requires flexible production and logistics (Kiefer et al. 2023).

Intralogistics is crucial for managing the production supply and disposal. However, the planning of logistics processes in the chemical industry is very complex due to the chemicals to be handled. A study by Kiefer et al. (2023) has identified requirements that must be considered for planning logistics processes in producing specialty chemicals, e.g., avoiding contact between employees and chemicals. That can be ensured by supplying production using tanks and pipelines, which eliminates manual transportation processes. However, frequently used stationary tanks are not flexible enough due to long cleaning times when changing raw materials and high regulatory requirements. This results in a conflict between ensuring safety and making logistics more flexible. One possibility to address this conflict is the implementation of tank containers (e.g., 20-foot containers). These are easy to replace when the raw material changes and only the pipelines need to be cleaned. This results in less downtime compared to stationary tanks and enables a flexible response to changes in demand while guaranteeing employee safety. For these reasons, this paper

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aims to enable the usage of tank containers in producing specialty chemicals through systematic planning of the supply strategy for the tactical planning horizon. In the chemical industry, this tactical planning horizon usually is one to twelve months. It includes planning tasks such as container management, planning of tank farm occupancy, or production order scheduling. Therefore, simulation and mathematical optimization methods are used to plan the logistics processes. First, the chemicals stored in the tank containers must be selected. Then, the influence on the processes that still have to be carried out manually must be evaluated. This applies particularly to general cargo container management, as the chemicals' properties significantly influence it. For example, a chemical can require more general cargo containers (GCCs) than those stored in a tank despite a smaller quantity because of regulatory requirements like storage in specific containers.

In this context, the paper is structured as follows: Related work is presented in Section 2, followed by Section 3, where a framework for planning the usage of tank containers will be introduced. The developed framework is evaluated regarding a real-world use case. Section 4 includes an overview of this use case. Afterward, the framework's methods are presented in Section 5 and Section 6 and evaluated regarding the use case. Finally, Section 7 summarizes the results obtained and provides an outlook.

2 RELATED WORK

Various methodological approaches and concepts are applied in planning and controlling logistics processes in the chemical industry. Frequently used solutions are production planning and control systems. These systems enable users to utilize plants, including the individual components, optimally based on the production orders and, thus, operate them economically (van den Houten et al. 2023; Georgiadis et al. 2019). In addition to scheduling plant occupancy, the chemical industry has methods for assigning employees to individual plants (Awad et al. 2022). However, these systems do not sufficiently consider logistics processes. Although they determine the demand for raw materials, they do not provide detailed information about the logistics processes, such as transportation, storage, or weighing. However, knowledge about these operations is essential, as every raw material is subject to different regulatory requirements, such as storage in cold conditions or specialized containers. In addition, the logistics processes to be carried out manually are subject to stochastic influences that these scheduling systems do not consider. Consequently, the mentioned algorithms are insufficient to plan the production supply with tank containers. The arrangement of production orders, determined by the scheduling algorithm, should rather provide the foundation for further logistics planning.

Operations research methods are widely used for planning logistics processes. Due to their advantages, mainly simulation and mathematical optimization methods are used. While optimization provides accurate solutions, simulation is often used for highly complex systems with stochastic influence to properly evaluate a decision's effects. However, mathematical optimization is limited due to the effort required to model the various influencing factors of logistics processes and the resulting long calculation times for holistic planning. Simulation, on the other hand, is a suitable method for evaluating the interrelationships between different subsystems. In addition to representing complex interdependencies, simulation enables a simplified consideration of stochastic influencing factors and the temporal behavior of complex systems (Tekin and Sabuncuoglu 2004). For example, Poeting et al. (2017), Clausen et al. (2012), and de Keizer et al. (2015) combine mathematical optimization and simulation. The authors explain the use of both methods by considering the interactions of the different subsystems and stochastic influencing factors in the process. The sole use of mathematical optimization would lead to an impractical calculation effort. Therefore, in the case of Poeting et al. (2017), a parcel transshipment terminal, the optimization method plans the timeslots of the incoming trucks and allocates them to the gates, in order to use the advantages of optimization and make an optimal decision for deterministic factors. The results obtained with the optimization are evaluated with simulation, which enables stochastic influences and interactions between different subsystems to be considered with a lower computing time than the optimization could achieve for these factors. The study's results demonstrate a successful application of this combination approach. Based on this experience and the comparable initial situations (optimization of tank occupancy and evaluation of the optimization on the holistic logistics system with simulation), this paper also uses a combined approach.

Regarding the methods of simulation and optimization, a systematic literature review based on the guidelines of Durach et al. (2017) is conducted. This aims to evaluate the common use of the methods for logistics planning in the chemical industry. The following search terms and combinations of these are used to identify relevant sources: "simulation“, "optimization“, "logistic*“, "supply chain“, "chemical industry“, "chemical*“, "specialty chemical*“, "production planning“ and "performance chemical*“. For this purpose, publications from the databases Scopus, Web of Science, Google Scholar, and Science Direct are examined. In addition, only publications in English and German and publications newer than 2017 are considered to ensure the actuality.

After full-text analysis, 25 results emerged. The evaluation of the results shows that the methodological approaches of simulation and optimization are rarely used in chemical logistics. The focus of these publications is on planning the supply chain rather than on planning the local production supply. For example, Eskandari et al. (2024) use mathematical optimization to plan a network for the hydrogen supply chain by formulating their problem in a Mixed Integer program. Other publications address the implementation of digital twins. However, these focus on production processes and process engineering and aim to improve production output. Logistics is not considered a strategic influencing factor in these publications. One example is the publication by Schmidt et al. (2021), which deals with a digital twin of the production process for COVID-19 vaccines. The aim is to validate the production scale and optimize processes. There is no consideration of the effects on the logistics processes for production supply or how logistics processes can be optimally planned. The literature analysis shows a considerable need for more publications on logistics planning for production supply in the specialty chemicals industry (Marques et al. 2020). However, some publications regard logistics as an essential strategic factor, highlighting the need for coordinated planning of logistics processes (Demmer 2020). Furthermore, no paper was found that considered the planning of using tank containers for the production supply. Therefore, a framework that combines simulation and optimization will be developed in the following sections. The aim of this framework is to decide whether and how tank containers should be combined with GCCs. The following section outlines the architecture and the technical implementation, including general principles and framework modules.

3 ARCHITECTURE OF THE COMBINED FRAMEWORK

A framework that combines simulation and optimization has been developed to support planning concerning the tactical planning horizon. This includes planning the supply type for an existing infrastructure consisting of tank container storage areas, including pipelines to the production sites. The architecture of the developed framework is shown in Figure 1. The main idea is a sequential arrangement of exact optimization and simulation, which will help to evaluate the plausibility of the optimization results with simulation (VDI 3633 Part 12 2020). Due to the tactical planning horizon, which allows longer computing times to obtain solutions that are rather accurate than fast, the framework is not limited to heuristics or metaheuristics. Furthermore, simulation is applied instead of including stochastic decision variables in the optimization model to allow better user interactions, visualizations, and implicit calculation of transport distances in the warehouse by the simulation software. For a better understanding of the architecture and the interactions of the components, a description of an experiment can be explained as follows:

First, the production data of the plants are implemented in the optimization module. These data include the production orders, their start and end times, the quantities of required materials, their costs, and the supply types. Afterward, the user must manually compile data. This includes the number of available tank container storage areas, the length of the observation period, or the selection of materials that can be stored in a tank. The optimization module generates an optimal tank storage occupancy plan based on the input data. The solutions are stored in a database. In addition, a user interface was generated, which shows the user a visually presented solution. Next, several simulation runs must be determined to

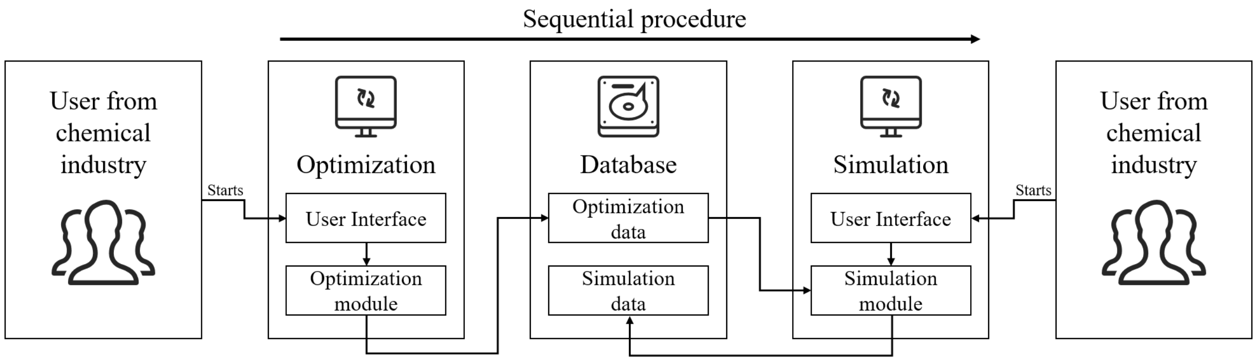

Figure 1: Architecture of the planning procedure.

guarantee the stochastic safety of the solution. The user can enter the number of replications by a further user interface. The parameterization of the simulation model is automated. Therefore, only the database needs to be adjusted. After manually inputting the number of required replications and the scenario under consideration, the user starts the simulation runs. Here, an interface has been implemented that reads the current data from the database and temporarily stores them in the simulation model. After each simulation run, the results and key performance indicators (KPIs) are calculated within the simulation model and saved in the database or an Excel list. The experiment's results include the logistical process times, the system's average GCCs, the number of direct interactions between employees and chemicals, and the employees' utilization in the individual simulation runs. This enables the analysis of key performance indicators (KPIs) using statistical methods and allows conclusions to be drawn about the influence of the supply type. Figure 2 shows a schematic representation of the described process flow. This procedure can be repeated as often as required to generate possible solutions, from which decisions can be made.

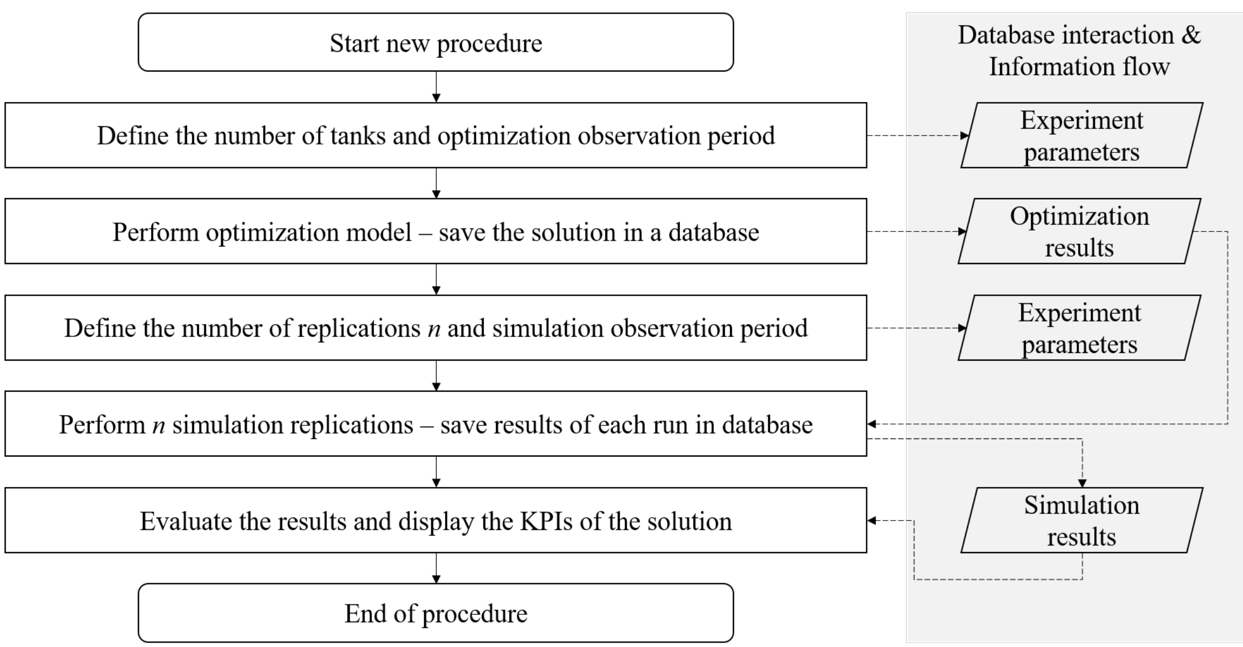

Figure 2: The procedure for planning the use of tank containers.

Next, the developed use case is evaluated using a real-world use case. This use case is based on a chemical company, which plans to use tank containers as a supply type. Therefore, Section 4 presents a detailed use case overview.

4 USE CASE

This section presents a real-world use case for evaluating the framework for tactical planning problems, such as the use of tank containers. The subject of investigation is a chemical company that wants to store specific raw materials in tank containers. The aim is to determine, whether tank containers should be used as well as which raw materials should be stored in the tanks and for how long, depending on the production orders. The observation period in this use case is one year because the company plans its production one year in advance. However, due to uncertainties in production planning, this period can be adjusted as required depending on the application. Furthermore, the company intends to increase employee safety, reduce direct contact between employees and chemicals, and – ideally – reduce supply costs. The company has two spots available for this purpose, which already have pipelines to the production plants. Moreover, the capacity of the tank containers is specified as 25 m^3. The company is considering storing nine raw materials in tank containers due to their chemical properties. Table 1 lists the raw materials that can be stored in a tank container for the presented real-world use case. In addition to the material identification, the table shows the type of GCC (Intermediate Bulk Container, barrels etc.), the costs of cleaning the GCCs, and the capacity of the tank or GCC regarding material properties, such as density in kg/m^3.

Table 1: Materials, the corresponding GCC type, GCC cleaning costs and capacity of a tank and a GCC for the materials.

Material	GCC type	GCC cleaning costs in €	Capacity in kg	
			Tank	GCC
0	C	000.00	28,750	950
1	B	245.56	19,725	702
2	B	245.56	19,725	702
3	B	245.56	21,250	702
4	B	245.56	19,725	800
5	A	406.95	21,375	200
6	D	288,66	19,550	711
7	E	000.00	28,000	500
8	B	245.56	21,250	702

It can be seen that Material 0 and Material 7 are delivered in single-use GCCs. Furthermore, it is assumed that the empty single-use GCCs will be returned to the supplier without cleaning. For this reason, no costs are charged for cleaning the GCCs. Based on the production orders, it will be determined which material will be stored in these tanks and how the identified selection will affect the GCC management. This is particularly interesting, because only a certain number of GCCs of each type are available. In addition to the respective production order quantities, the logistics processes to be carried out manually significantly influence the number of GCCs needed. The developed framework will not be limited to this use case, but clarifying the application helps to evaluate and will guide through the modeling process.

5 OPTIMIZATION

The first part of this section presents the mathematical model for selecting the raw materials to be stored in a tank container to make the decision as accurate as possible and build a solid simulation foundation. Furthermore, the model is expected to deliver good results within a tolerable time regarding the planning horizon. The presented model is applied to the use case, and analysis results are shown.

5.1 Optimization Model

Before formalizing the problem as a Mixed Integer program, the notation outlined in Table 2 must be introduced. Here, every parameter can take any non-negative real value. These parameters represent the integer quantities of time intervals (T) in the observation period, tanks (K), and considered materials (R). Variables are defined as follows: $t \in \{0,...,T\}$, $k \in \{0,...,K\}$, and $r \in \{0,...,R\}$. Moreover, $p \in \mathbb{N}$ is the number of time intervals for cleaning the pipelines.

Table 2: Input parameters for the optimization model.

a_{tr}	production jobs	g_r	material costs per kg in a tank
γ_r	material costs per kg in GCC	h_{kr}	capacity of a tank
d	provision costs of a GCC	b	handlings costs of tank exchange
$\hat{k}_r$	capacity of a GCC	c	cleaning costs of a pipeline
$\hat{c}_r$	cleaning costs of a GCC	$\hat{y}_r$	material waste costs per kg

The GCC capacities vary depending on the materials' density. The main goal is to decide between storing the materials in a GCC or a tank container. To model this decision, four binary variables are introduced: e_{tr} indicates whether a GCC is used for material r at time t, u_{tkr} represents whether tank k is used for material r, l_{tr} characterizes the arrival of material r at time t, and y_{tk} shows whether tank k is cleaned at time t. Furthermore, the integer value s_{tr} specifies the number of GCCs needed at time t for material r depending on the volume of production jobs and capacity. The real-valued f_{tkr} indicates the tank level of tank k at time t with material r. The cost function that is to be minimized is the following:

$$\overbrace{\sum_{t=1}^{T}\sum_{k=0}^{K}\sum_{r=0}^{R} y_{kt}\cdot(c+f_{t-1,k,r}\cdot\hat{\gamma}_r)}^{(i)\text{ pipeline cleaning}} + \overbrace{\sum_{t=1}^{T}\sum_{r=0}^{R} l_{tr}\cdot(b+h_{kr}\cdot g_r)}^{(ii)\text{ tank container exchange}} + \overbrace{\sum_{t=1}^{T}\sum_{r=0}^{R} e_{tr}(\gamma_r\cdot a_{tr}+s_{tr}(\hat{c}_r+d))}^{(iii)\text{ GCC usage}} \quad (1)$$

Costs arise in three different cases: (i) if the raw material in a tank container changes, the pipeline must be cleaned, (ii) if more of the already stored raw material is required, the tank container will be exchanged, and (iii) if GCCs are used for production supply. For the selection of the supply type, the following constraints need to be fulfilled:

$$\begin{aligned}
&\min && (1) && \\
&\text{s.t.} & s_{tr} &= e_{tr}\frac{a_{tr}}{\hat{k}_r} && \forall\, t=1,...,T; \quad r=0,...,R && (2)\\
&& f_{tkr} &\le k_{kr} && \forall\, t=1,...,T; \quad k=0,...,K; \quad r=0,...,R && (3)\\
&& f_{tkr} &= (f_{t-1,k,r}-a_{tr}\cdot u_{tkr}+l_{tr}\cdot h_{kr})(1-y_{tk}) && \forall\, t=1,...,T; \quad k=0,...,K; \quad r=0,...,R && (4)\\
&& y_{t-1,k}\left(\sum_{n=\max\{t-p,1\}}^{t-1} y_{nk}-p\right)+p\cdot y_{tk} &\ge 0 && \forall\, t=1,...,T; \quad k=0,...,K && (5)\\
&& v_{tkr} &\le u_{tkr} && \forall\, t=1,...,T; \quad k=0,...,K; \quad r=0,...,R && (6)\\
&& l_{tr}+e_{tr} &\le 1 && \forall\, t=1,...,T; \quad r=0,...,R && (7)\\
&& u_{tkr}+y_{tk} &\le 1 && \forall\, t=1,...,T; \quad k=0,...,K; \quad r=0,...,R && (8)\\
&& u_{tkr}+e_{tr} &\le 1 && \forall\, t=1,...,T; \quad k=0,...,K; \quad r=0,...,R && (9)\\
&& \sum_{r=0}^{R} l_{tr} &\le 1 && \forall\, t=1,...,T && (10)
\end{aligned}$$

$$\sum_{k=0}^{K} f_{tkr} \cdot (1-e_{tr}) + a_{tr} \cdot e_{tr} \geq a_{tr} \qquad \forall\ t=1,...,T; \qquad r=0,...,R \quad (11)$$

$$u_{tkr} \geq \frac{1}{\max_{k,r}\{k_{kr}\}} f_{ktr} \qquad \forall\ t=1,...,T; \quad k=0,...,K; \quad r=0,...,R \quad (12)$$

$$u_{tkr} \leq u_{t-1,k,r} + y_{t-1,k} \qquad \forall\ t=1,...,T; \quad k=0,...,K; \quad r=0,...,R \quad (13)$$

$$\sum_{r=0}^{R} u_{tkr} \leq \Phi \qquad \forall\ t=1,...,T; \quad k=0,...,K \quad (14)$$

$$\sum_{k=0}^{K} \left(\sum_{r=0}^{R} u_{tkr} + y_{tk} \right) = T \qquad \forall\ t=1,...,T \quad (15)$$

$$l_{tr},\ e_{tr},\ s_{tr} \in \{0,1\} \qquad \forall\ t=1,...,T; \qquad r=0,...,R \quad (16)$$

$$u_{tkr},\ v_{tkr} \in \{0,1\},\ f_{tkr} \in \mathbb{R}_{\geq 0} \qquad \forall\ t=1,...,T; \quad k=0,...,K; \quad r=0,...,R \quad (17)$$

$$y_{tk} \in \{0,1\} \qquad \forall\ t=1,...,T; \quad k=0,...,K \quad (18)$$

As mentioned above, (2) specifies the required number of GCCs of a raw material r at time t, whereas (3) and (4) indicate the tank fill level within the capacity. Constraint (5) models the non-usability of a tank during the cleaning process, and (6) ensures that an exchange of a tank container can only happen if a tank is in use. Furthermore, (7), (8), and (9) ensure that a material can only be stored in either a tank or a GCC at the same time. In addition, it cannot be stored in a tank during cleaning. Moreover, an exchange tank container can only transport one material (10), the production orders need to be served (11), and a tank can be filled with material if and only if it is used (12). Additionally, a tank is either filled with the material from the period before or it is filled with a new material after the tank is cleaned. Optional constraints restrict the number of tanks that can be used for a raw material at a time to an integer Φ (14) or that every tank needs to be used or cleaned (15). Constraints (16) – (18) specify the domains of the considered decision variables. In the following section, the developed model is applied to the use case described in Section 4.

5.2 Optimization Results

In this section, the mathematical optimization model from Section 5.1 is applied to the use case described in Section 4 without the optional constraints (14) and (15). Gurobi 11.0.1 is used within Python 3.12 for testing, as it can be directly applied to the optimization model from Section 5.1, being able to handle products of up to two decision variables. Furthermore, the optimization model uses two hours as the time discretization, as the company can exchange an empty tank container with a full tank container with the same material within two hours. Moreover, the other logistics processes (tank cleaning, order demand, etc.) can also be calculated at two-hour intervals, and this discretization reduces the calculation time. The mathematical model was verified and validated before being applied to the use case. This includes checking whether the model exchanges tank containers, cleans the pipelines, or only uses GCCs for high pipeline supply costs. The verification and validation process did not identify any issues, and all constraints worked as intended to ensure that GCC and tank usage are separate events in the solution while serving the production order. Next, the use case was carried out. Therefore, the observation period is one year. In the use case, a gap for the objective bounds of about 9 % was achieved after 48 hours of computing time. The results for the occupancy strategy are given in Figure 3 with dark colors, indicating that the respecting pipes are cleaned. The proposed solution initially fills the tanks with Materials 4 and 5. This seems reasonable, as the GCC costs for Materials 4 and 5 are quite high. Therefore, storing the materials in tanks saves costs. This also explains why these materials are stored in tanks for quite a long time from the beginning (more than 1,500 and 2,500 intervals, respectively). After the initial storage strategy, the pipelines are cleaned, and the empty tanks are replaced with Material 6 in Tank 1 and Material 3 in Tank 0. Material 4 is also

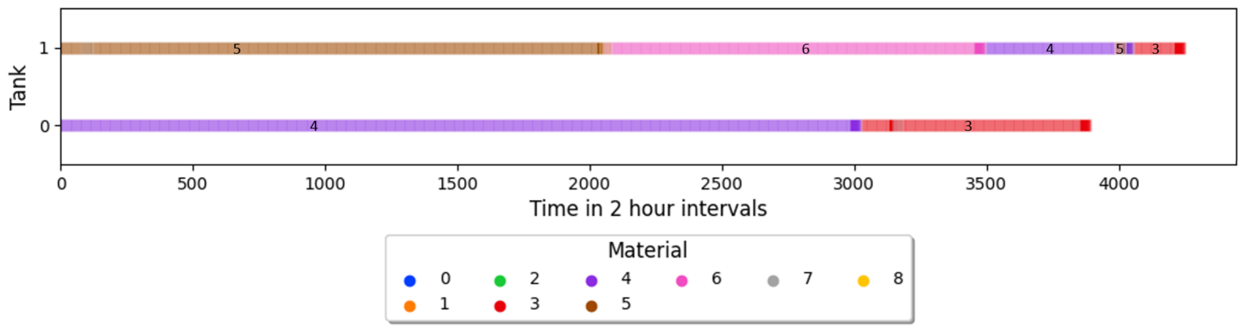

Figure 3: Occupancy of the tank containers.

stored in Tank 1 shortly after Tank 0 was emptied with Material 4. In contrast, Materials 0 and 7 are never stored in tanks, as the costs of storing them in GCCs are quite low and it could cost more to store them in tanks. In Section 6, the influence of the raw materials selected for storage in tank containers is evaluated using simulation regarding GCC management.

6 SIMULATION

Following the investigations concerning the mathematical optimization, the influences of the selected raw materials for the tank containers on the holistic logistics system have to be analyzed using simulation. The focus here has to be on the effects on container management and the reduction of direct contact between employees and chemicals. This section introduces the conceptual structure and the procedure for developing the simulation model. Furthermore, the simulation results for the use case are presented and analyzed.

6.1 Simulation Model

The simulation model used within the framework is created with AnyLogic 8.8.5 according to the procedure described by Rabe et al. (2008). AnyLogic combines three different modeling methods and examines various levels of abstraction in a single model. The developed simulation model uses discrete and agent-based modeling and includes several agents.

A detailed goal had to be defined in the first developing step, including the task specification. Furthermore, key performance indicators (KPIs) were defined to evaluate the different scenarios of the production supply in two variants; only with general cargo and with a combination of general cargo and tank containers. These KPIs include the number of GCCs in the system by container type, the number of interactions between employees and chemicals, resource utilization, and logistics process times. The required data were collected, prepared, and clustered according to VDI 3633 Part 1 (2014) in technical, organizational, and system data to reach the goal. For example, the company's layout, number and type of GCCs, or the capacity of the logistics facility are technical data. Organizational data included process structures such as the employees' shift schedules or allocation of resources for tasks. Afterward, the system data were prepared, including the production orders, for the simulation.

In the next step, a conceptual model was developed. Here, the source is receiving the raw materials and their subsequent storage. The finished products' outbound flow and reusable GCCs cleaning are the sink. After the conceptual model of the entire production process was created, the entire process was divided into individual processes. These particular processes were represented as event-driven process chains, which subsequently simplified the implementation of the logistics processes in the simulation model. Based on this, the simulation model consists of the agents main (the central agent), production building, logistics building, container cleaning building, forklift, packing material, production order, cleaning order, general cargo container, tank container, production order management, and material. Furthermore, an automated parameterization was included in the model. Thus, only the database needs to be adapted when scenarios change.

The executable model's correctness is observed by validation and verification techniques (VDI 3633 Part 1 2014). Validation in dialogue took place with experts from chemical companies. For this purpose, the formal model, the model behavior, and the prepared data were explained. Comments and corrections from the experts were incorporated into the formalization of the simulation model.

6.2 Simulation Results

Regarding the defined use case from Section 4, two scenarios are evaluated using simulation. In the first scenario, no tank containers are used, and GCCs supply the raw materials manually. In the second scenario, a part of the production supply is handled by tank containers, with the occupancy of the tank containers implemented based on the optimization results from Section 5.2.

As in the optimization study, a representative year regarding the order volume was defined for the simulation. Stochastic effects play a significant role in the model, where each simulation run is characterized by unique initial conditions influenced by shifts, manual logistics processes, and more. Consequently, analyzing the transient phase to evaluate the simulation experiment independently from this initial period is crucial. Figure 4 shows the GCCs in the system for the current situation over the first two months of the observation period. According to Welch (1983), cyclical behavior appears from the 28th day onwards, defined as the end of the transient phase.

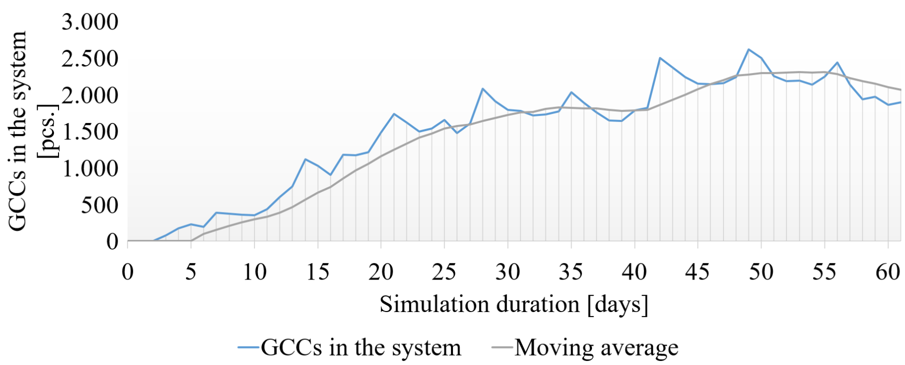

Figure 4: Transit phase of the simulation model according to Welch (1983).

In addition to defining the transient phase, the number of replications was determined using confidence intervals. Therefore, the number of GCCs in the system and the process times for the logistics processes were recorded and analyzed. Due to this model's long observation period of one year, a replication number of ten can guarantee stochastic reliability. Based on this, ten simulation runs were conducted for each scenario. The following evaluation of the simulation results includes the respective mean values from all ten simulation runs per scenario.

Figure 5 shows the GCCs in the entire logistics system of the company over the simulation duration in months. Furthermore, a differentiation is made between the two scenarios shown in the diagram. The blue line represents the first scenario without the supply-type tank containers and the orange line represents the second scenario with a combination of GCCs and tank containers. As mentioned above, the optimization study's results (Section 5.2) are implemented in the second scenario (orange line).

The implementation of tank containers has reduced the amount of GCCs in the logistics system. This is particularly noticeable at the end of the observation period. From month 1 to month 12, the demand could be reduced by up to 1,500 GCCs, a reduction of almost 30 %.

Furthermore, the simulation provides a detailed look at a single GCC type. Therefore, we look at GCC type B, which is used for Materials 3 and 4 (see Table 1). In addition, these materials are selected

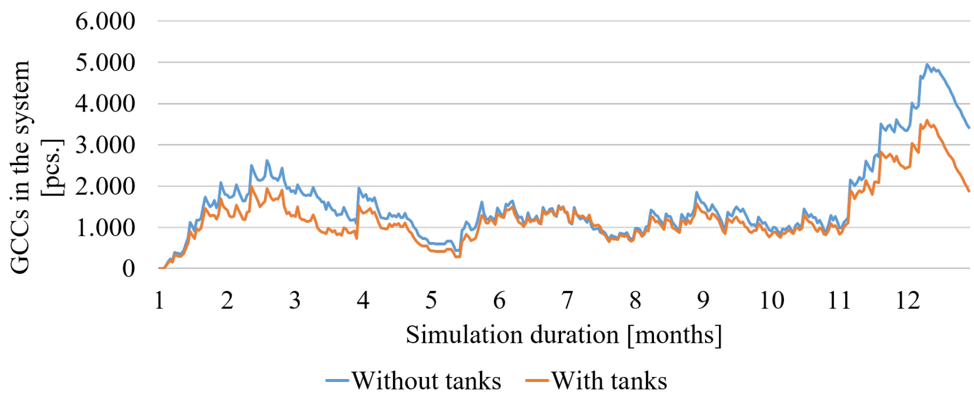

Figure 5: GCCs in the system.

for storage in a tank container (see Figure 3). The required GCCs of type B are shown in Figure 6. The evaluation of these results also shows how significantly storing raw materials in tank containers influences the demand for GCCs of a specific type. For example, the demand is reduced by almost 75 % in the third month.

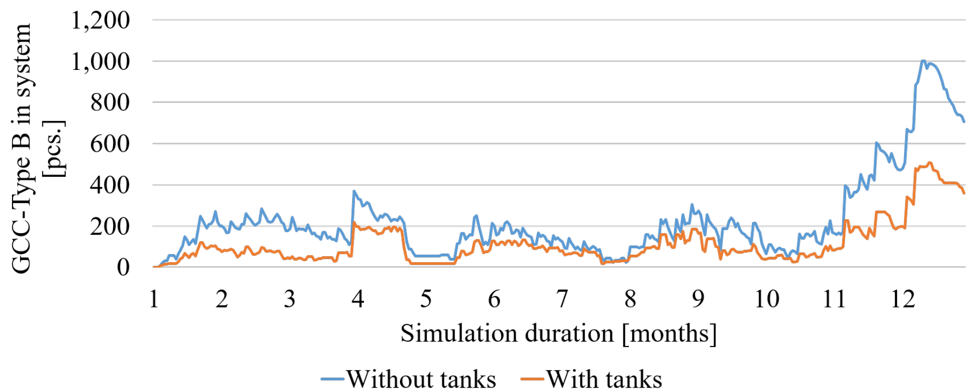

Figure 6: GCCs of type B in the system.

Additionally, direct interactions between employees and chemicals are reduced significantly. In this use case, the interactions include storing the chemicals, transportation to and from the production site, bundling on trailers, and transporting the bundled GCCs to the cleaning and disposal site. While the first scenario without using tank containers involved over 90,000 interactions, these were reduced by around 25 % to less than 68,000. In addition to the results presented in this paper, the simulation model enables the determination of the ideal number of employees per shift or the analysis of resource utilization. This includes utilizing employees or specific sites for batching or cleaning processes. For example, Figure 7 shows the different supply strategies' impact on the utilization of the logistics employees in the scenarios. Therefore, the study assumed three shifts of eight hours in a seven-day working week. The results show that employee utilization also decreases with the use of tank containers. This also reflects the observations of the reduced interactions between employees and chemicals.

7 CONCLUSION AND OUTLOOK

This paper presented a framework that combines simulation with mathematical optimization to plan the supply of raw materials for producing specialty chemicals. A real-world use case was introduced to validate

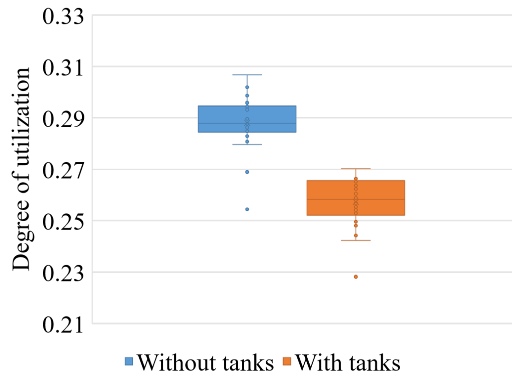

Figure 7: Utilization of logistics employees.

the developed framework, which investigates two supply scenarios. In the first scenario, the production supply was held only with manual logistics processes and GCCs. The second scenario used tank containers directly linked to the production plants in addition to GCCs. The raw materials stored in the tank containers were selected using mathematical optimization, and the simulation evaluated the influence of this choice on the entire logistics system. The results showed that using tank containers significantly influences the interactions between employees and chemicals. Furthermore, the simulation provides essential information about the GCCs required for each type. It showed that the demand for different containers continuously varied over the observation period due to changes in the raw materials in the tank containers and the production orders. Consideration of stochastic influences made planning the number of needed GCCs possible. The results underline the advantages of combining simulation and optimization in a framework, as it allows the evaluation of several possible solutions in multiple independent simulation experiments. Further research will focus on integrating stationary tanks into the planning framework and developing generally usable simulation blocks for logistics processes and buildings. This enables chemical companies to apply the framework more easily, with only the infrastructure changes needing to be implemented. Furthermore, the simulation model for the use case is expanded in the next step. The aim is to evaluate the influence of the choice of supply type on the production buildings. In particular, the influence of a freight elevator on the production supply is currently a bottleneck for the company being considered.

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