Logistics Simulation in the Chemical Industry

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1. Introduction

Since several years, the manufacturing industry has to deal with increasingly difficult conditions such as a growing number of product variants, smaller lots and reduced batch sizes. At the same time the development from a supplier to a buyer market, where (besides prices) product quality and delivery dates also play a major role in the sales process, puts increasing pressure on production logistics. In this context, the objective is to achieve an economic production process with a high level delivery service, low inventories, and short lead times. These classic challenges, at times with slightly varying target variables, can be resolved or at least simplified with computer-aided analysis of production and logistics processes. One widespread technology for the analysis of production processes is computer simulation. Simulation helps to increase the transparency of the structures and operating rules within a production system and it allows a quantitative assessment of the efficiency of material and information flows. Some typical areas of application are bottleneck analysis, balancing of production and buffer capacities, support of investment decisions, and issues around dispatching, scheduling and sequencing of production lots and orders.

2. Areas of Application for Logistics Simulation in the Process Industry

The methodology of logistics simulation was first used with success in the early 1970s in the discrete manufacturing industry—mainly in the machine and the automotive industry. The origins of simulation technology date back even further and many significant developments were initiated by military applications. Some historical information can be found in Nance (1993). In the machine industry and even more in the automotive industry, simulation has for many years become a well-established methodology and very few investment decisions are made without it. On the basis of the success in the discrete manufacturing industry, several companies in the process industry began using material flow simulations in the late 1980s and early 1990s, initially for bottleneck analysis and decisions on plant design, cf. Watson (1997). However, it turned out that simulation software tools and the results from other industries could be used in the process industry only after some modifications. Günther and Yang (2004) give several examples on the specific complexity of processes in the process industry: there are constraints to batch sizes, shared intermediates, changing proportions of input and output goods, production of by-products, limited predictability of processing times and yields, blending and mixing processes, use of multi-purpose resources, sequence and usage dependent cleaning operations, finite intermediate storage, product specific storage devices, cyclical material flows, usage of secondary resources such as energy or steam, complex packaging and filling operations, detailed quality controls. These and more restrictions and side factors distinguish production planning and hence modeling of production processes in process industry from discrete parts manufacturing as it is found, e.g., in the automotive industry.

Hence, it took the software industry longer to provide tools for logistic simulation that are capable of covering these extended requirements and could be used in the process industry environment. During the 1990s the process industry in Germany started several joined initiatives to enhance discrete event simulation packages to their needs. Today, several large companies in the chemical industry make use of the benefits of simulation.

The areas of application for material flow simulation and the simulation activities of the users in the chemical industry do not only cover the various sections of the supply chain on different levels of detail but also the entire life cycle of technical systems, including the organizational procedures. Simulation is used in the planning and engineering phase, during system ramp-up, and in the operational phase, depending on the task and the objective of the investigation as indicated in Figure 1.



Figure 1: Level of detail and timeline of simulation application

This article strives to give some insights in the use of simulation in the chemical industry. Accordingly, the remainder of this paper is organized as follows: Section 3 is providing a short overview on the typical steps in a discrete event simulation project. Section 4 presents three examples on the application of simulation in the process industry.

The examples highlight the great scope of possible applications starting at the planning (or re-engineering) of the replenishment in a multi-site production network, supporting decision-making within a plant engineering process on production and tank capacities and finally being part of the daily lot scheduling process in the context of material requirement planning (MRP) in collaboration with enterprise resource planning (ERP) systems such as SAP R/3.

Section 5 discusses some experiences with expenses and benefits of simulation use and section 6 will provide some technical information on available simulation software. The concluding section 7 summarizes some of the aspects and contains statements on possible future lines of development.

3. The Simulation Process in Manufacturing and Logistics

In the simulation literature there are several process models for simulation studies, see e.g. Sargent (1982), Nance and Balci (1988), or VDI (2000). Whereas these process models deviate in several details they all do have four typical steps in common:

- 1. Problem analysis and definition of objectives
- 2. Data acquisition
- 3. Model design, implementation, and validation
- 4. Application of the model

Of course, these steps usually are not processed in a linear order. There are rather loops and iterations. The acquired data might lead to new insights in the problem and hence cause a shift in project objectives. The model implementation may cause additional data requirements and the application might show that there need to be model modifications. And depending on the scope and the objectives of the model the extend of the four steps may differ significantly. However, there are characteristics for each step of a simulation study which are briefly discussed in the following subsections.

3.1 **Problem Analysis and Definition of the Objectives**

Every logistic simulation needs to be preceded by the analysis of the investigated problem. The customer's needs and expectations are defined within one or several project meetings. One of the main issues to be answered is whether simulation is the appropriate methodology to tackle the specific problem. In this context, general advice is rather difficult, but some criteria for the use of simulation are a sensible cost-benefit ratio, a lack of alternative methods, e.g., analytical-mathematical models, stochastic

influences with regard to resource availability or incoming orders etc.. Besides the assessment of simulation as the suitable method it is also crucial that the project objectives are stated as precisely as possible and that there is a clear understanding that these objectives may well be achieved by means of simulation. In this context it should be made clear that simulation is not a substitute for a sound planning process. Simulation does not *develop* concepts but it is a good means to assess them.

3.2 Acquisition of Required Data

After clarification of objectives and methodology the relevant data to create and run a simulation model is defined and compiled. In general, the required data can be divided into technical data, organizational data, and system load data. The technical data includes information about the system topology and layout (e.g. the number of tanks, batch processing units and pipes for the simulation of a chemical plant), material flow data (e.g. transportation via pipe, bulk, container etc.), performance data (e.g. the input and output information for the processes), and usage times of equipment and production facilities, storage capacities (e.g. the capacity of the tanks) and availabilities (including cleaning or set-up times of tanks or processors). Organizational data includes production strategies (e.g. the campaigns to run), rules for product manufacturing (e.g. the dispatching of orders in a specified process step) and information about staffing of processes and the working time models. Information about production orders, quantities, and deadlines as well as product data (e.g. formulas) are described as system load data. The period of time considered within the model (e.g. the production schedule of one year), the level of detail, and the quality of the data to be recorded depend mainly on the complexity and requirements of the task at hand.

Detailed acquisition of data before the actual model is created leads to increased transparency of the procedures and thus usually has its own intrinsic value. However, the effort to collect and prepare data for a simulation study should not be underestimated. As a rule of thumb, the data collection sums up to one third of a simulations projects time budget. In supply chain studies, where data of several production sites may be needed, the expenses for data collection may even be higher.

3.3 Model design, implementation and validation

Modeling in the context of this article means the implementation of an actual or a planned production or logistics system in a computer model. In this respect, modeling has some similarities to a software engineering project and as within a software project it is good practice to specify or design an application before the implementation starts. Hence, a (good and experienced) simulation analyst creates a conceptual model and a formal model before actually implementing a computer model. It contains decisions on the

elements, structures, rules and stochastic influences in the actual or planned system which have to be considered important for the projects objectives and therefore need to be part of the model. Typical decisions during the process of conceptual modeling are for example which sites or product lines may or may not be included in a supply chain model. Or decisions on the level of detail of a plant model are explained (e.g., whether the maintenance staff is explicitly modeled or not). In general, it can be said that a system should not be modeled as exactly as possible but as exactly as necessary to tackle the respective task – and the root for this decisions is conceptual modeling.

While the conceptual model is still on a non-simulation-expert level and understandable for the simulation expert as well as any project engineer, the formal model is pushing on step further towards an expert level. Here, data structures and algorithms may be designed in detail before in the final modeling step the formal model is transformed into a computer model.

The implemented model must be tested with regard to correctness and completeness. Therefore, i.e. to validate the model and ensure the credibility of the simulation results, suitable scenarios with a broad spectrum of different events are reproduced with the model and compared to reality (or to expectations on reality). A model validated successfully can then be used for several systematic experiments (or as part of other applications, e.g. as part of a MES).

Modeling and validation require the close cooperation of all parties involved in the project. Further success factors in simulation modeling include adequate planning experience, special experience with simulation tools, and the ability to think in abstract structures.

3.4 Application of the model

The way of applying a simulation model depends on the purpose it has been created for. A model for supply chain or plant design usually is created to support engineering decisions. Hence, the application of such a model means to conduct several series of experiments where design parameters of the considered system are modified. Design parameters may be production or warehousing capacity of a site, the allocation of products to sites and warehouses, or lead times for products in a supply chain studies. In a study to support plant design, the capacity of tanks or of productions processes may be subject of the experiments. The results of the model experiments are presented using appropriate key figures. Common key figures are throughput times, output per time unit, tank and resource utilization over time, service levels etc. Most simulation software tools present the results in tables or graphs such as line graphs, bar diagrams, pie charts, or Sankey diagrams. Other important information about the behavior of the simulated systems is provided by process animation. This visualization of the procedures during a simulation experiment provides additional transparency and reliability for planners and simulation experts when they are evaluating the model behavior and the results.

If a simulation model is used as part of an MES to evaluate production schedules and support daily operation the presentation of simulation results quite often is integrated in the MES environment. The planner might not even see or know the simulation model itself. There might be a feature such as "assess order schedule" within the MES which starts a simulation experiment. Details on this and on the other ways of application will be illustrated by the examples in the next section.

4. Case studies

As sketched out initially simulation can be used at different points in time of a production systems lifecycle and with a different scope (cf. Figure 1). Considering the lifecycle and the scope, the three case studies described in this section may be classified differently, from supply chain to plant level and from planning to daily operation

4.1 An example of simulation in Supply Chain Design

In general, supply chain simulation can be used along the life cycle of supply chains, that is from supply chain design to support of supply chain operation. In supply chain design, simulation models can support supply network design (decisions on the location, ramp-up or shutdown of production or warehousing sites) as well as the adjustment of control parameters such as safety stock at different nodes, production lot sizes, transport options etc. An overview on the potential of supply chain simulation based on a survey of 80 articles can be found in Terzi and Cavalieri (2004).

The case considered in the following is about a small study which was carried out using a discrete-event simulation tool and specific add on to model supply chains efficiently. Even though it is a rather small example it highlights the level of modeling and decisions under consideration in a supply chain simulation study. The objective of the study was to assess different replenishment strategies for a product processed in Europe and refined at three different sites in China. The transportation is carried out by cargo vessels. The analysts had to evaluate three alternative strategies:

- Direct replenishment of the tanks at the three Chinese production sites based on safety stock and forecasts on customer demand
- Using a concept of floating stock, i.e., the product is shipped in Europe without already having a request for replenishment from China. Instead, the anonymous "floating" stock is assigned to an order while it is on the passage somewhere between Europe and China
- Employing an additional intermediate tank system in Malaysia

Due to stochastic demand in China, stochastic production yields in Europe and some stochastic variations in transport times between the two it was decided to support the decision between these alternatives by means of simulation. The structure of the simulation model is shown in Figure 2.



Figure 2: Example of a highly aggregated supply chain model

The resulting stock at the different locations of the supply chain was displayed in charts as the example in Figure 3. Additionally, the total stock, the different transportations costs and the costs for using the resources in Malaysia were taken into account and finally let to an recommendation for the floating stock concept together with a specific combination of decision variables.



Figure 3: Example of a highly aggregated supply chain model

4.2 An example of simulation in Plant Design and Engineering

Whereas the model objects in supply chain simulations are whole plants or transport relations between plants, in plant engineering the simulation objects are on a far more detailed level. Typical elements of the modeling process on this level are process units such as reactors, tanks, pumps, filling stations and discrete transport units such as bulk containers, bigbags etc. In the presented case study, the objective was to investigate whether a tank farm for a given product had the right capacity to ensure the continuous supply of downstream processes on site (captive use) as well as the satisfaction of external customer orders. Figure 4 is giving an overview over the modeled structure. On the left hand side there are two processors continuously producing a product. While there is on average a constant production rate, the effective daily yield is significantly fluctuating due to tolerances within the process, maintenance activities etc. Figure 5 indicates those variances in production output for the first 15 days of the simulation period. The amount requested by customers is known several days in advance but is also subject to substantial variations as can be seen on the right hand side of Figure 5.

The two processors are delivering the product via pipes into one of several tanks in a tank farm. Each tank has parameters such as capacity or cleaning time. From the tanks the product is either delivered to processes on site (captive use) or to customers based on given customer orders. Additionally, it may be stored in two external buffers. In that case there are transportation moves from the tank farm to one of the external buffers (in case of over-production) or from the external buffer to the tank farm (in case of shortages in production) induced.



Figure 4: Screenshot of a combined supply chain and plant simulation model



Figure 5: Daily production output of simulated process and customer orders

Even though this model does not cover several production sites such as the preceding example it still requires a significant amount of input data:

- Capacity of upstream and downstream production facilities including average and deviation in day yield, maintenance policies, shift models and availability
- Customer orders per day and per transport medium (IBC, Bigbags)
- Number and capacity of tanks including rules for cleaning, re-filling etc.

Based on these and other inputs the simulation model is providing several outputs. Main results are

- A chart for each tank showing the quantity held over time (see Figure 6)
- The service level in terms of customer orders fulfilled on-time
- The number of transports classified by transport type (transport of customer ordered material or transports from and to external buffers)

Figure 6: Simulated Quantity in Selected Tanks

In considered case study the simulation results had significant impact on investment decisions within the tankfarm and on the agreements negotiated with the service partners responsible for the external buffers.

In particular results on tank capacity are a typical output of simulations on the plant engineering level. It could be argued that these results may be obtained without simulation as well and this is true as long as the stochastic impact on supply and demand is within certain boundaries. As soon as the facility needs to be able to handle stochastic supply and demand with significant variations static calculations are reaching limits. These limitations become even more critical if a multi-product process is analyzed as it quite often is the case.

4.3 An example of simulation in Plant Operation

The main difference between the third and the two other case studies is that the simulation model here is applied as tool for daily production planning. In that sense the model may well be considered as part of the MES for the production. Its main purpose is to assess order schedules (calculated by optimization algorithms either within the model or handed over by an ERP system). Whereas the structure of the model and the data requirements may be very similar to a simulation model used for the support of the engineering process, the way the data is getting into the model needs to be completely different. During the engineering process it usually is sufficient (and quite often the only way) to collect and compile the required data manually in spreadsheets or even to enter it directly into the simulation model. If the model is to be used for daily order dispatching in a production environment it needs to have several interfaces to other software tools: orders need to be supplied from the ERP system (e.g. from SAP R/3), the current status of the production needs to be fed into the model (coming from a shop floor control or monitoring system), and there needs to be a user interface that is easy to handle for the staff in charge of production control. A generic framework for the architecture of suchlike systems is shown in Figure 7.

Figure 7: Scheme of an MES-integrated simulation application

Of course there are many planning solutions offered by vendors of MES or APS (advanced planning systems), cf. Stadtler and Kilger (2005). The great advantage of a simulation based solution is the almost unlimited flexibility in modelling the production processes. Thus, even schedules for very complex production environments can be assessed. However, the main expenses in these projects quite often do not stem from the modelling process itself but rather from adjusting the user interface, implementing the interfaces to other applications, establishing a stable data transfer and the roll-out and test of the system. Hence, the scale of an MES integrated simulation project tends to be five to ten times larger than the typical engineering support project.

5. Benefits and Expenses of Simulation Projects

The expenses of simulation projects vary considerably depending on the type and the area of application. Apparently, this is the case if one looks into such different applications as engineering support and MES functionality. However, even simulation studies for engineering support can comprise several days or several months. The proportions for the different phases of a simulation in the overall project expense can be defined as follows: definition of the objectives: 10-20%, data gathering and preparation: 25-40%, modeling: 30-50%, validation: 10-25%, experiments and analysis of the results: 20-30%. Such as in other fields of manufacturing or software engineering there is no standard procedure for evaluating the cost-benefit ratio for logistic simulation. Some general advantages are an improved understanding of the processes and the

possibility of taking specific, effective actions. Incorrect planning can be identified at an early stage and the planning risk is minimized. However, the benefits can only be quantified for specific projects. Nevertheless, a cost-benefit ratio of 1:4 to 1:6 appears to be realistic. In investment projects for new plants, a cost-benefit ratio of 1:20 and more could quite easily be achieved.

In spite of the potential benefit, the possibilities of logistics simulation are often not fully exploited. Some reasons are a lack of knowledge about the basic methodology and and the available simulation tools, the fact that simulation models are rarely deployed more than once, and simulation investigations are often integrated into the planning process too late.

6. How a Simulator works

There are many different simulation techniques for modeling different types of complex systems (e.g., process simulation, finite element methods, system dynamics). Essentially, discrete-event simulation has become established for use in logistic issues. Specific software tools (simulators) are needed for the implementation of simulation studies. The corresponding market has grown over the years and now offers a wide variety of programs, e.g., simulation tools eM-Plant, Witness, or AutoMod. An overview over commercial simulation packages is provided in a biannual series by Swain (2005). There are significant differences in the level of maturity of, both, the tools and the software vendors, and in the technology that is used for modeling and optimization, the possibilities of integration with other software systems, and the costs for license and software maintenance.

The discrete event simulation tools of the leading software vendors usually can be used to cover all the fields of applications discussed in this article. Some may have a focus more on detailed material handling, while others offer better support on modeling supply chains. And there are significant differences to what extend interfaces are supported, a feature which is getting important if a simulation model is going to be integrated with other applications. An analyst in the process industry who is planning to use simulation and who is looking for the right software should specifically pay attention to the following issues:

 Since almost all of the discrete event simulation tools have their roots in modeling discrete manufacturing processes, some of them still do not offer the objects an analyst in the process industry needs. Every simulation package will offer typical objects of discrete manufacturing plant: machines, buffers, parts, vehicles, etc. But to model chemical processes objects such as tanks, pipes, pumps, reactors etc. should be provided by the simulation tool. Similarly, if the simulation tool mainly is used for supply chain studies, it should offer objects suitable to model on a higher level. A pipe or a packaging machine are not quite the appropriate objects to start the modeling of a worldwide supply chain. Here, it takes rather objects such as site, transport relation, depot etc.

- A discrete event simulation tool considers nomen est omen discrete events at discrete points in time. Typically, in a discrete event simulator items such as parts are moving through the modeled system changing their state, e.g., when they enter or leave a machine. A reactor in the process industry does continuously produce a certain output. This is something a discrete event simulator is not really made for. One approach to model continuous output with a discrete simulator is by "slicing" the output in discrete portions, e.g. by using a part to model a certain amount of the reactors yield. This can be very costly in terms of computational performance if the slices are too small. If the slices are too large the simulation may loose accuracy. Another approach for continuous modeling is not to use moveable objects such as parts but rather model changes of reactor processes by state variables and counters. This may be a bit less intuitive but it usually leads to increased speed of simulation experiments in combination with sufficient accuracy. However, an analyst should be aware of both approaches and carefully look into performance limitations of the considered simulation package.
- The integration of a simulation application into an MES- or ERP-environment requires several interfaces. The simulation package needs to be "open" in the sense that it can easily connect to other IT systems and that other IT systems easily can connect to it. Possible interfaces are TCP/IP or ActiveX for telegram exchange, ODBC as database interface, or an interface to a programming language such as C++ or JAVA. These interfaces are also a prerequisite for a sensible way of exchanging data with an ERP system as SAP R/3 because usually the data exchange with such a system is implemented via one of those ways. The degree of support for the different interfaces can be very different from simulation package to simulation package.

7. Developments in the Field of Logistics Simulation

At present, the trend is moving from the analysis of individual production and logistics systems towards the optimization of entire production networks, that is, the optimization of the distribution to different production locations taking account of the procurement and distribution chain as indicated by the remarks on Supply Chain Simulation earlier in this paper. However, in particular for these applications there are some challenges in the basic work of providing consistent and coherent data describing the processes at different sites which most likely are located in different countries.

Another perspective for production simulation is automatic capacity utilization optimization of multi-product systems. As discussed, this task may be very difficult because of the many different variables and boundary conditions. In an environment integrating optimization and simulation, the optimizer systematically varies the important

decision variables in an external loop while the simulation model carries out production planning with the specified variables in the internal loop, cf. Günther and Yang (2004). The target function, for example total costs or lead times, can be selected as required. The result of optimization is a detailed proposal for the sequence of the placed orders.

It finally may be stated that the use of discrete-event simulation on different decision levels even though state-of-the-art is still slightly underrepresented in the process industry. However, since the technology has proven itself in an increasing number of cases in the past couple of years, there seems to be some promising potential for further successful applications.

8. Literature

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