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A. Simulation Tools and Their Application in Chemical Manufacturing I

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Simulation tools and models are becoming more and more important in the fields of process development and design, process parameter optimization or in the evaluation of process interaction and their dynamic simulation. Not only can they be instrumental in creating cost transparency and ultimately reducing costs or shortening time to market, but they are also able to significantly accelerate progress in process development or lead to the identification of optimization potentials. The three lectures demonstrated the step-by-step use of a mass, energy and cost flow model, showed the application of simulation tools with varying level of detail at different stages of process design and further discussed the possibilities of using dynamic simulation within chemical production.

Keywords: Chemical manufacturing · Cost optimization · Industrial chemistry · Simulation tools · Time to market

Efficiency Engineering: Cost Reduction Through Modeling of Manufacturing Costs

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In process development individual process steps are optimized for product quality and yield. Optimizing the investment costs is the main driver in the planning of a production plant. As a consequence, less attention is paid to operating costs, which become relevant when the plant is up and running. This often results in unnecessarily high operating costs and an increase in cost of ownership.

Costs for supplying raw materials and energy and for treatment and disposal of waste materials may be as high as 80% of the total manufacturing costs of a chemical product. With industry margins thinning, the ratio of supply and disposal costs to profit deserves attention; a 10% profit margin and 10% disposal costs means that saving half of the disposal costs would increase profits by 50%.

Efficiency Engineering is a unique methodology based on mass and energy balancing for reducing production costs in the chemical and pharmaceutical industry. In contrast to the traditional approach of optimizing single process steps, efficiency engineering focuses on the overall production costs.

Example 1: Optimization of Water Management (Fig. 1)

Based on measurements the water consumption was reduced, the efficiency of the wastewater treatment improved, and the environmental problems solved.

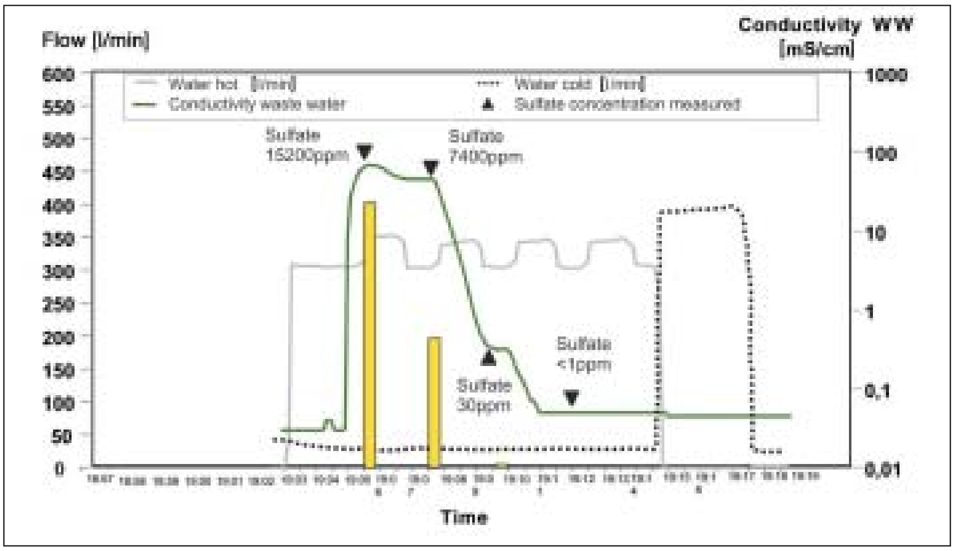

Fig. 1. On-line measurements of water consumption (hot and cold) and wastewater quality (conductivity and sulfate concentration) were used to improve a batch washing process.

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Example 2: Air is Not Free of Charge (Fig. 2)

In the planning of a new production plant the operating costs were assessed to be EUR 4.05 per 10'000 m^3 of solvent exhaust. Due to the high operating costs expected the exhaust flows were optimized.

Example 3: Modeling Manufacturing Costs of a Chemical Production Plant

The assessment of the supply and disposal costs of a chemical production plant was performed and the data were used to build the mass, energy and cost model (Fig. 3). The total costs per 1089 kg of dry product was CHF 9938 (16% disposal costs). The model was challenged together with process specialists and cost savings of more than 2000 CHF per batch were identified.

Conclusions

Efficiency Engineering is a proven and valuable approach to meet current as well as future challenges and opportunities for cost reductions while simultaneously lowering the environmental impact. The methodology was applied successfully for:

- Cost reduction of process equipment and production plants
- Modeling and optimization of manufacturing sites
- Planning of production extensions and new production facilities
- Assessment of product costs
- Benchmarking
- Facility management
- Improvement of eco-efficiency (ISO 14001)

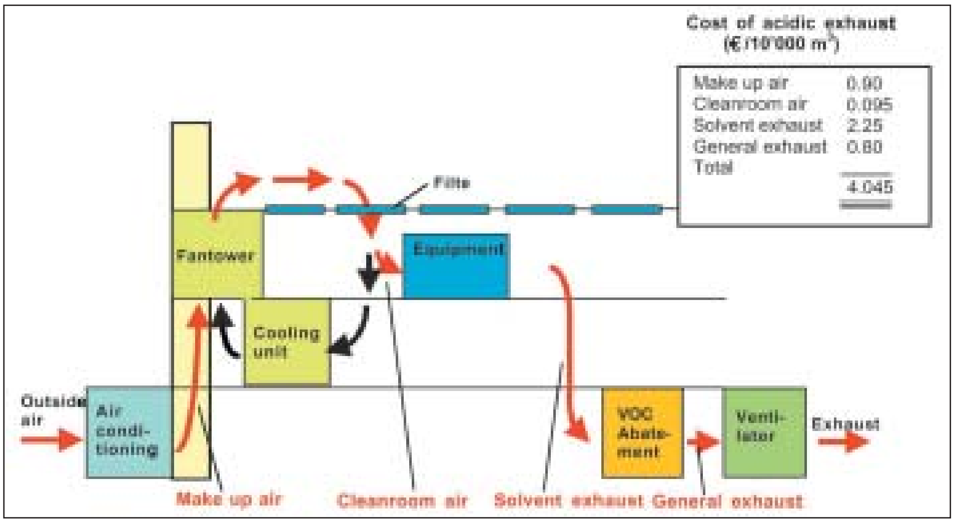

Fig. 2. Calculation of operational costs for the treatment of solvent exhaust from a process equipment located in a cleanroom environment. The costs are based on local prices for electricity, water and wastewater at yearly average climatic conditions in Central Europe.

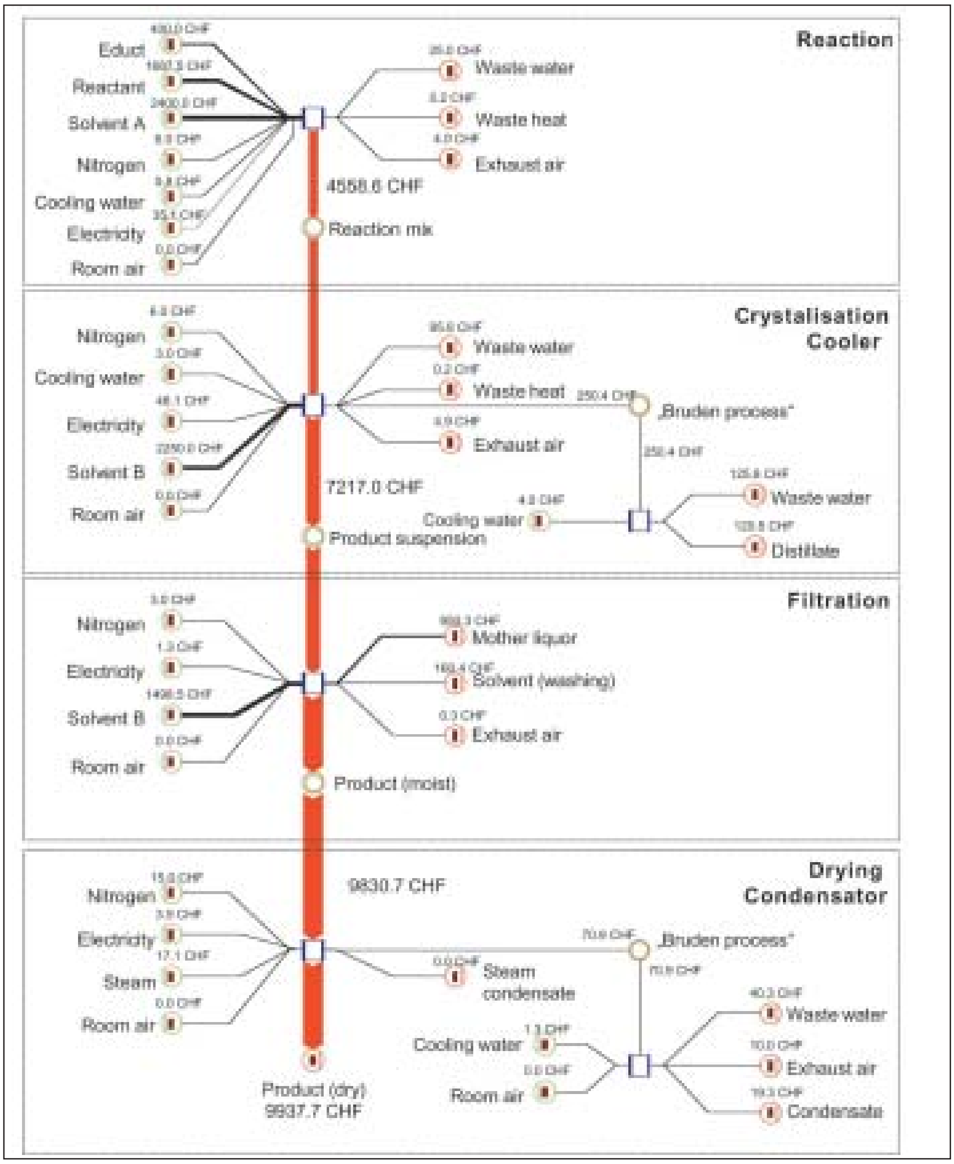

Fig. 3. Mass, energy, and cost flow analysis of a chemical synthesis. The illustration shows cost flows only. All supply and disposal cost flows for each process step are allocated to the final product costs (vertical arrow). The thickness of the single cost flow lines is proportional to the overall costs.

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The Use of Modern Simulation Tools for a Shorter Time to Market

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In the times of globalization speeding up the development process is more and more important to achieve or maintain market leadership. Simulation programs can be a valuable tool to reduce costs, prevent wrong decisions and to ensure more planning reliability.

Fig. 4 shows the typical dilemma of projects in new business development. Whereas money is not an issue at the start of the project, the knowledge about the critical factors relevant for a fast and cost efficient realization is very limited. The necessity to come to decisions without the full information will last most of the time until the end of the project. Unfortunately corrective actions become more and more expensive as the end of the work approaches. Simulation tools could help to obtain more information, before spending too much money for a second class solution.

The application of simulation tools of differing complexity was presented. As an example for a fine-grained simulation tool the application of Computational Fluid Dynamics (CFD) calculation for the improvement of a separation device for the removal of solid particles from liquids was shown. Starting from this case several key success factors for the use of simulation tools were identified:

- Defining a clear aim: Is simulation really the solution to your problem?
- Identify the relevant processes (chemical, economical, physical *etc.*) and concentrate on the relevant ones

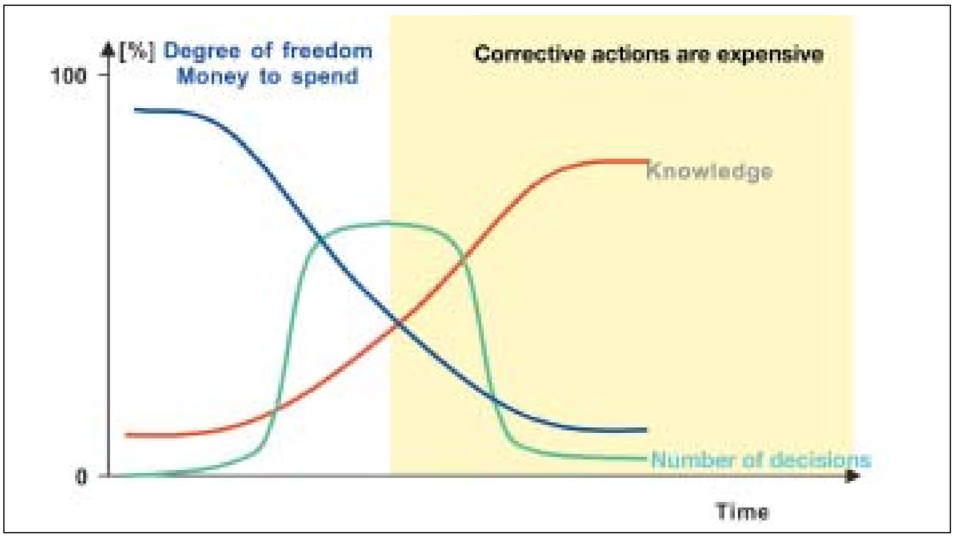

Fig. 4. The trap of knowing few details and making a lot decisions.

- Define the boundary conditions (*e.g.* flow of material, heat, the compositions of the streams)
- Be aware of non-physical boundary conditions (cost, utilization of equipment, abilities of workshops *etc.*)
- Assure the assistance of simulation professionals to verify your model and draw the right conclusions from the obtained results

As a second example the application of a whole set of simulation tools in the new business development process was shown. The scale-up of a chemical process involving the reaction of ketene with a ketone was significantly accelerated through the application of simulation tools. Fig. 5 shows three of the important factors for the development of new products. Choosing the right product, bringing it fast to the market obeying low production costs is the key to success.

For the chemical process under investigation one reaction step was up-scaled the standard way from 1 l to 1 m^3 to 10 m^3. The second reaction step was up-scaled directly from lab-scale to production scale. It could be shown that the costs related to the implantation of the chemical steps in production could be reduced by a factor up to 20 using only 20% of the time. This impressive achievement was reached through the application of simulation software in combination with the verification through lab-scale experiments.

A summary of the advantages of simulation tools yields the following points:

More knowledge: Identification of relevant processes is accompanied by a learning process

Speed up: Planning reliability is enhanced at earlier development stages

Visualization: Hidden aspects are made visible

Storage: Models compress data obtained by measurements

Control: Models could be applied to control complex systems

Enhanced Safety: Hazard studies could be performed safely

Training: Models allow safe training of operators

The author thanks the members of the Computer Aided Process Engineering Department of the Lonzagroup and the Department of Mixing- and Reaction-Engineering of Siemens Axiva.

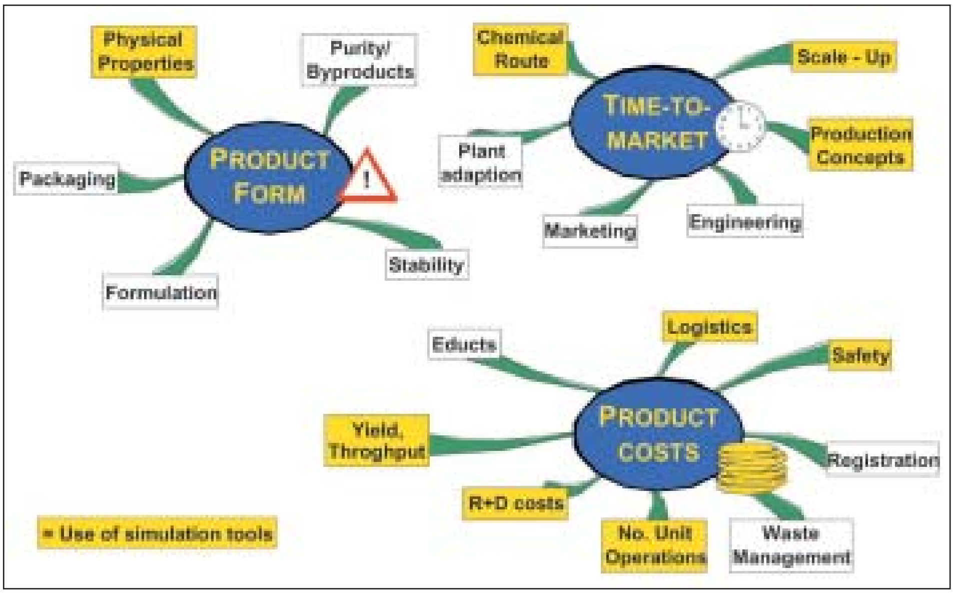

Fig. 5. Possibilities to improve the introduction of new chemical products

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Application of Dynamic Simulation for Optimization of Chemical Processes

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In addition to the chemical and technical optimization of production processes, a third area dealing with the synchronization of a process can be identified. This field deals with the problem of how vessels, isolation units, dryers, regeneration systems and tank farms work together and how they influence each other.

Within F. Hoffmann La-Roche Ltd. we use simulation software in order to obtain a better understanding of interactions within our chemical processes and to identify potential for capacity increase with a minimum of investment. With the help of simulation tools different potential solutions can be visualized in a short time and the results can be used to support the decision-making process of an investment.

A central information source for understanding a process is the usage of Gantt Charts where the correlation between equipment used and time needed is drawn up. Gantt charts drawn up with classical methods like paper and pencil, spreadsheets or MS project give only information about the static behavior of a process. But when for *e.g.* the time dependency of a tank level *versus* time is of interest, the classical methods can give only limited answers. Using simulation tools the dynamic behavior of the process is taken into account and influences to the process are reflected in the resulting Gantt chart.

In order to understand the influence of the auxiliary systems like tank farms, regeneration systems, number of containers available *etc.* we need a dynamic simulation of the process in a computer model in order to open another window for a new perspective to our process.

The data base for a model consists of five elements: ACTIONS describe the unit operations needed to produce a compound. RESOURCES and DURATION are information about where it is done and how long it will take to do the action. QUANTITIES are for *e.g.* amounts of solvents going into or out of the action. LOGICAL RULES are the conditions driving the process.

With these data a model can be built up with the help of a simulation software. We use the software D3GO from BRIGHTRIVERS which offers a high flexibility for transferring the real process to a model and run simulations.

An example out of a project undertaken at Roche shows how dynamic simulation can help to identify process improvements.

The process (see also Fig. 6) has two major parts. In the first part the reaction is performed and after several operations the crude product is isolated. After dissolving the crude solid again the solution enters the sterile part of the process for final crystallization, isolation, drying and packaging to cans.

In addition to the main process there are processes that support production. These are, for example, the tank farm, a solvent regeneration unit, a separate water system and an autoclave needed to transfer cans, sample bottles and clothes to the sterile part of the process. The simulation model includes all these parts and also includes the special rules and interactions of these components that influence the main process and therefore the capacity.

When running the simulation of the existing process, a capacity of 138 to/a was identified. In Fig. 7 a zoom into the Gantt chart is drawn up. The bottleneck of the total process can be clearly identified at vessel R12-CRYS where sterile crystallization is undertaken. When looking at this line an interruption of 0.5 h for this critical part can be seen. This originates ultimately from the autoclave (R16-AUTO last line of Gantt) and the rules under which it is operated.

In order to increase capacity the sequence of the different parts running through the autoclave was changed. With this new rule simulation shows an increase in capacity to 141.7 to/a and no interruption on the critical line of R12-CRYS was found. This is an example of how capacity of the main process is influenced by supporting equipment. The increase in capacity was achieved by changing a rule with zero investment.

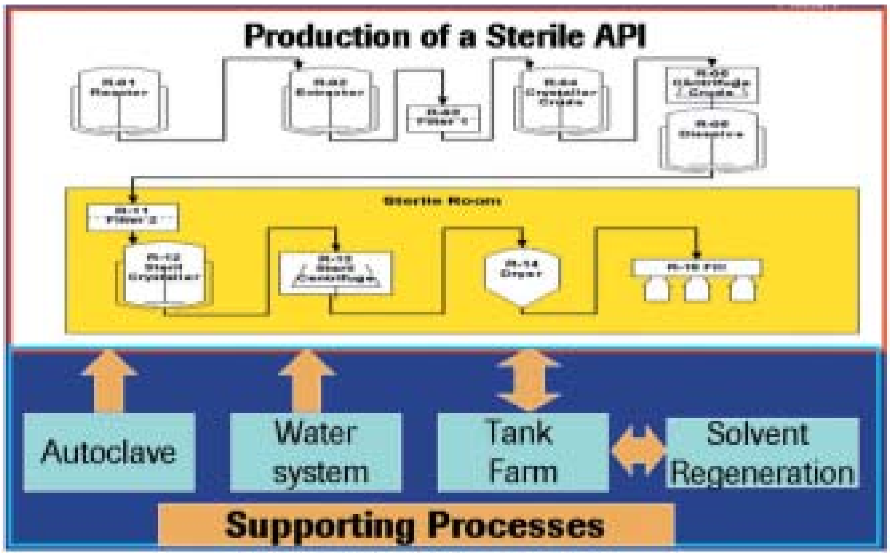

Fig. 6. Process example

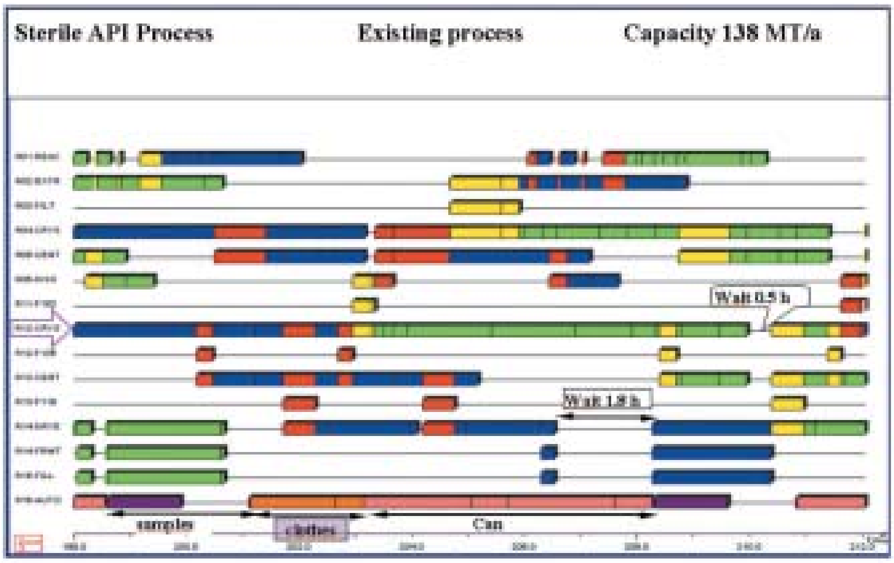

Fig. 7. Gantt Chart production process

A simulation model of a process can also be used to simulate the influence of equipment failure, for example, and the consequences and timelines occurring before the process has to stop. This provides valuable information for implementation of preventive steps in order to avoid an interruption.

Simulation models can also be used as part of the training activities of the employees working within the process. It helps to give them an overview of the production and clarify the interactions of the process they are working on. A central part is also to visualize the consequences of the worker's own behavior such as waiting too long before starting a certain action. The result of such a mistake can be shown online by implementing it in the model and obtaining the result within a few minutes. With this method effects on the capacity can be shown without doing it in the real process.

With the help of dynamic simulation we can obtain additional information about the interactions within a process, about the capacity of a process, the location of the first, second, third... bottleneck and the gaps in between. It also helps us to test proposed solutions and see the results within short time. Human resources can be focused on the current problems and we have also an additional source of information for making decisions on investment.

B. Simulation Tools and Their Application in Chemical Manufacturing II

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Simulations have various objectives, such as avoiding costly experiments in reality, the prevention of large-scale pilot production procedures, or the analysis of cases where critical situations are not accessible experimentally. In addition, they are useful for the identification of possible parametric sensitive processes, allow the prediction of hazardous situations, but also provide an effective chemical process training for operators and experts in a safe environment. The three lectures explained which methods of simulation are most practically used during the development of a procedure, showed the benefits of numeric simulation techniques in process safety, and highlighted the potential of simulations in training skilled workers in chemical operations.

Keywords: Process safety · Process simulation · Simulation tools · Simulation training

Dynamic Modeling for Batch Process Simulation: A Case Study and Software Tool Development

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Batch processes in the fine chemicals and related industries frequently involve multiple phases with mass and heat transfer in addition to the chemical reaction. They are rarely true batch operations and usually include the addition of at least one of the reactants over a period of time. A schematic diagram of such a process is shown in Fig. 8.

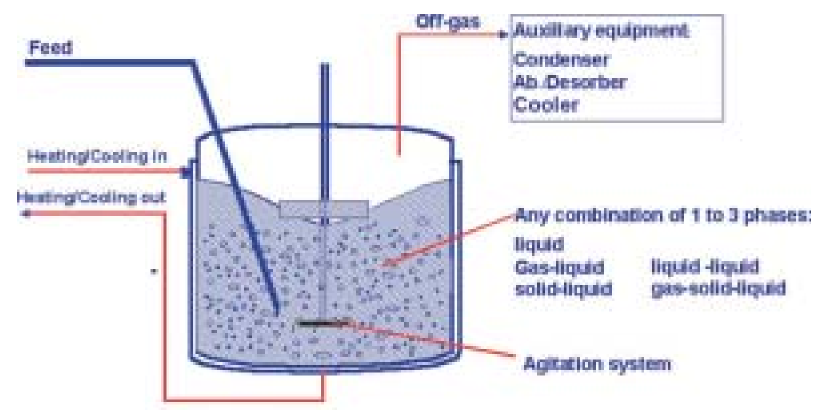

Fig. 8. Schematic of a typical semi-batch reactor

The output from these processes can be sensitive to changes such as the scale of operation, agitation or raw material properties. This is due to the effect on the relative rates of competing steps such as mass transfer and reaction. Such processes are characterized by being time-dependant. Detailed study of these systems requires dynamic simulation rather than the more common steady-state approach.

The use of this approach can be illustrated by considering an example where

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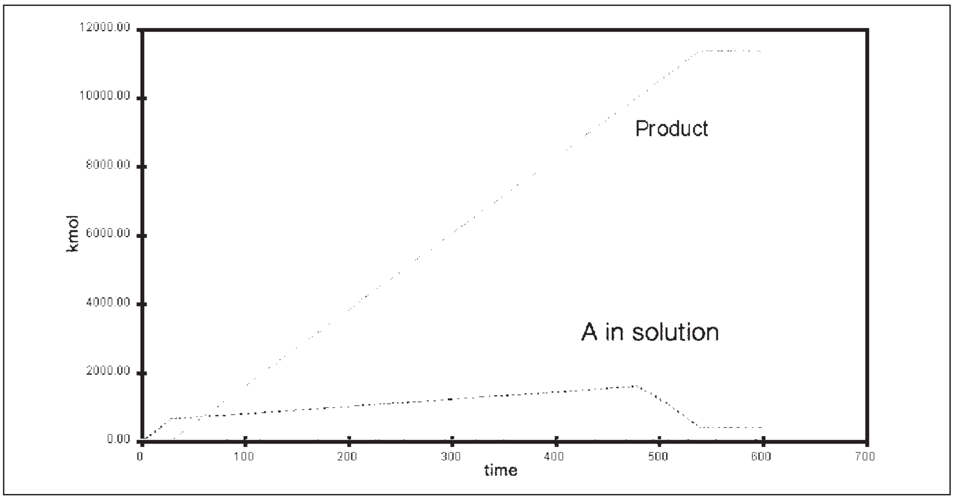

Fig. 9. Reaction profile for small particles

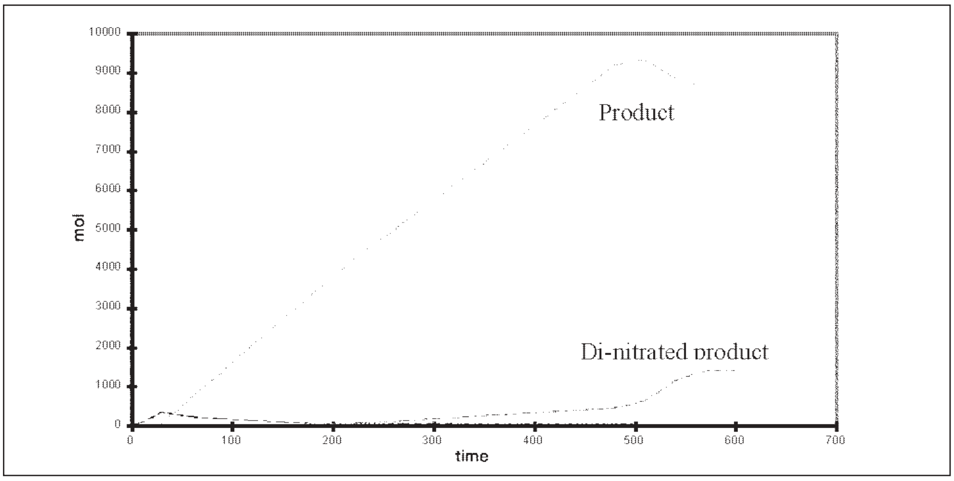

Fig. 10. Reaction profile for large particles

product quality problems were encountered in the manufacture of an agrochemical intermediate. The organic starting material (A) in the form of a solid was nitrated by co-addition with nitric acid into a solvent. A change in the particle size distribution of the starting material gave rise to a significant deterioration in product quality as a result of increased di-nitrated product. Dynamic simulation was applied to the problem, using an iterative process to develop and validate the model by estimating parameters, such as the mass transfer coefficient, to predict plant performance. The mass transfer rate is a function of particle diameter and the effect of increased particle size was to reduce the rate of mass transfer to the point where the quantity of A in solution was sufficiently low to allow the competing di-nitration reaction to become significant.

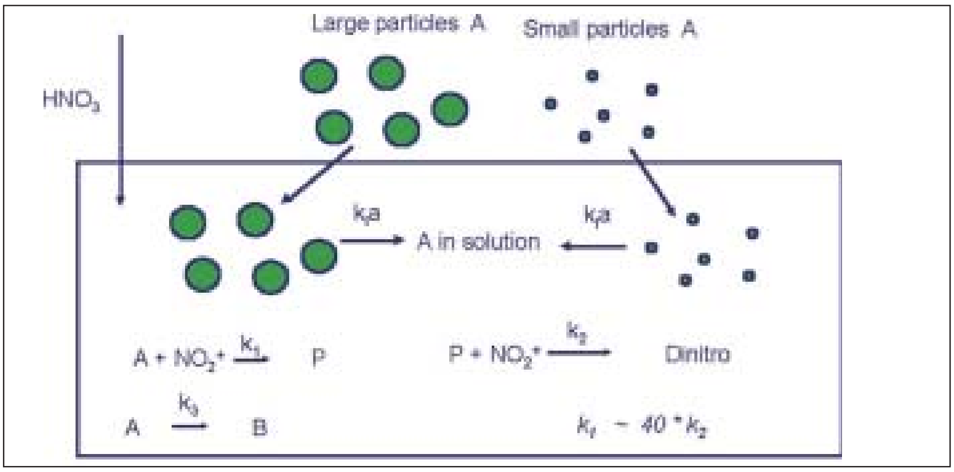

Fig. 11. Process scheme for nitration example

Use of this validated model led to modification of the operating conditions to overcome these problems and a restoration of the required product quality. Fig. 9 and 10 show the reaction profiles with 'small' and 'large' particles. The accumulation of the di-nitrated product can be seen in the latter case.

The systematic procedure followed in this and many similar examples, requires iteration around the proposed process mechanism and validation against measured data. It was found to be very useful to illustrate the process mechanism by means of a 'process scheme'. This is simply a pictorial representation of the physical and chemical processes involved and is shown in Fig. 11 for the example described above.

This example, and similar studies, highlighted the need for a general purpose simulation tool more suited to the needs of semi-batch reaction modeling for users who were not expert in the writing of differential equations. The requirements included the ability to model reaction kinetics, mass and heat transfer, vapor liquid equilibrium as well as addition and removal of reagents.

A software tool, DynoChem, was developed in Syngenta to allow simple input of reaction mechanisms and other process parameters using a spreadsheet. The spreadsheet is used to generate an input file for the model solver, which can be used by non-experts to run dynamic simulations of processes. In this way it was possible to extend the use of dynamic modeling to a wider process development population, helping to facilitate the interaction between chemists and chemical engineers. The consideration of the process scheme and development of the understanding of the chemical and physical processes involved is of great benefit in scaling up.

In a hydrogenation for example, careful data generation in the laboratory (including calorimetry) allowing quantification of the relative contribution of mass transfer, heat transfer and reaction kinetics in solution can allow scale-up into a well-characterized plant reactor without the need for piloting.

Since software development is not a core activity for Syngenta this package has since been commercialized by a company specializing in providing software to the process industries and DynoChem is now available from PFD of Dublin. They have provided many 'templates' for easier model set-up and included extensive help text. Further significant upgrades are planned which will include parameter fitting and optimization.

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Benefits of Numeric Simulation Techniques in Process Safety

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Numeric simulation techniques are now commonly used in chemical engineering. This technique is essentially used in two fields: (i) simulation of steady states for continuous processes and (ii) dynamic simulation of discontinuous processes. In the first application field, it allows chemical engineers to solve mass balances in processes with complex recycling schemes. In the second field it allows the prediction of the dynamic behavior of process steps. Both are essential in the scale-up of chemical processes.

These tools find also applications, even if less common, in the field of chemical process safety, where these applications can be classified in three different categories: (i) dynamic simulation of processes allowing the prediction of hazardous situations, (ii) solution of complex problems with partial differential equations as heat accumulation situations, (iii) didactic application to enable a good understanding of complex and non-linear phenomena.

Dynamic Simulation of Processes

Dynamic simulation is often used for the identification of kinetic parameters. In turn these are used in models to predict hazardous situations. This type of problem analysis is useful in cases where critical situations are not accessible experimentally. Of course in order to become reliable, this technique can only be applied when some rules are strictly followed. An example is given where the time constant of an industrial process was too high to follow the real process dynamics leading to a delayed alarm. During a malfunction of the cooling system of the reactor, the temperature increased, but due to the time lag, the inhibitor injection was triggered at too high a pressure and did not function. Thus a pressure release occurred. This could have been avoided if the process dynamics were studied by simulation techniques. This technique is also very useful for the identification of possibly parametric sensitive processes.

Dynamic simulation allows the identification of kinetic parameters even in case of complex reaction kinetics. An example is presented where the effect of measurement errors during DSC experiments allows the degree of confidence for the time to explosion under adiabatic conditions (TMRad) to be calculated. This study was performed using the methodology by ‘Advanced Kinetics and Technology Solutions’ (AKTS), which allows for a scientifically sound definition of safety margins.

Heat Accumulation Situations

The second field of application of numeric simulation techniques in process safety is the solution of partial differential equations as the y encountered in heat conduction problems. These problems arise when heat accumulation situations are to be analyzed. Some examples are storage, transportation or more generally handling of solids in physical unit operations. Numeric simulation allows the definition of safe operating conditions with tailored safety margins. Examples are given where the simulation of the heat transfer by conduction within a substance to be stored or transported allows safe conditions to be defined such as temperature of storage, size of package and maximum allowed duration for the rupture of cooling for an actively cooled storage.

Didactic Applications

The third field of application is didactics. Students – and people in general – are not accustomed to ‘think non-linear’. Numeric simulation techniques allows numeric experiments to be run that could never be performed in reality. The influence of operating parameters or kinetic parameters can be studied thoroughly in a short time and without danger. This was demonstrated on the example of autocatalytic decomposition reactions, which seem to behave in a rather unpredictable way. A systematic study of the influence of kinetic parameters allows students to get a feeling of how things work even under runaway situations.

Simulation Training in Chemical Operation for Skilled Workers

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As the complexity of business operation increases, it becomes more and more difficult to find means and ways to develop process knowledge for employees in chemical production plants. An effective chemical process training for operators and experts in a safe environment can successfully be reached by using state-of-the-art information technologies.

The *aprentas* production training department has implemented a process simulator to train apprentices, plant personnel and specialists in real-time processes.

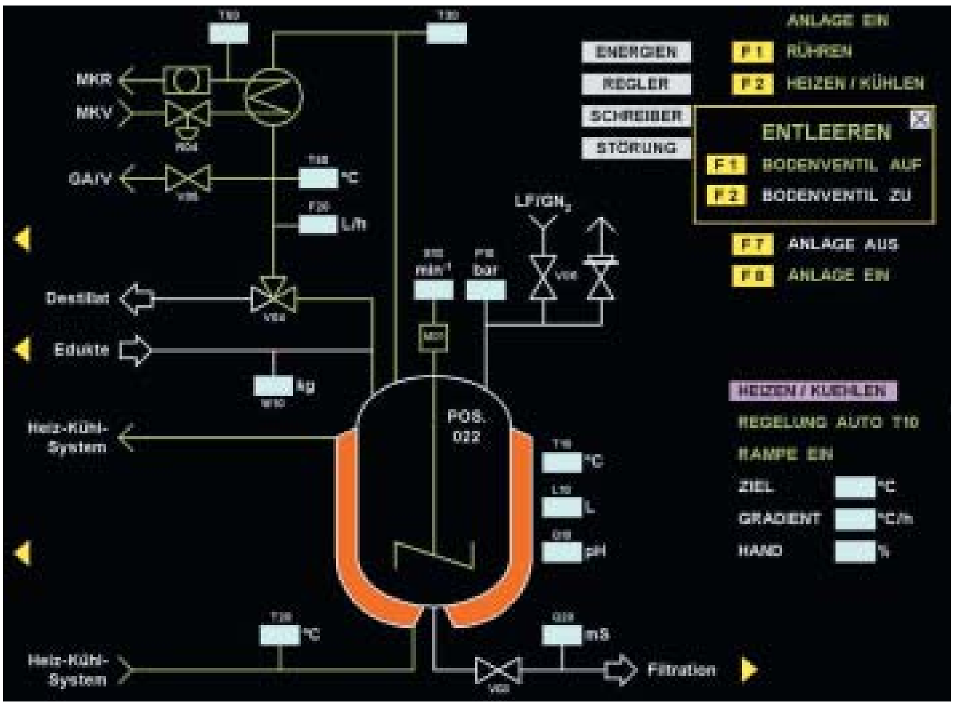

Fig. 12. Vessel presentation

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The Incident-Simulation-System (ISIS) is a flexible computer program for mathematical simulations of chemical processes, based on standardized hardware and software. It contains the necessary knowledge to calculate and simulate a wide range of physical and chemical operations. The simulation can be visualized in any specific kind of control panel. ISIS is written in G2, an expert software of Gensym Corp. This software is used worldwide in many areas, *e.g.* in process control systems in nuclear power plants. The ISIS software was developed by the SCI Company (Safety Consulting Institute, Binningen, Switzerland).

In practice, up to 15 trainees can be confronted simultaneously with a virtual reality of a chemical process or single aspects of technological operations (Fig. 12). The animated objects like the measuring instruments and recorders allow them to observe the course process flow and to control it in the same way as in reality. The implementation of various critical situations or system errors, like cooling failure during an exothermic reaction or the incorrect feed rate of a reactant by instructors, enables users to experience hazardous situations and to learn how to handle them. Furthermore, the possibility to observe any single sequence of complex processes improves the understanding of abstract chemical technical operations.

Fig.13. Simulation room

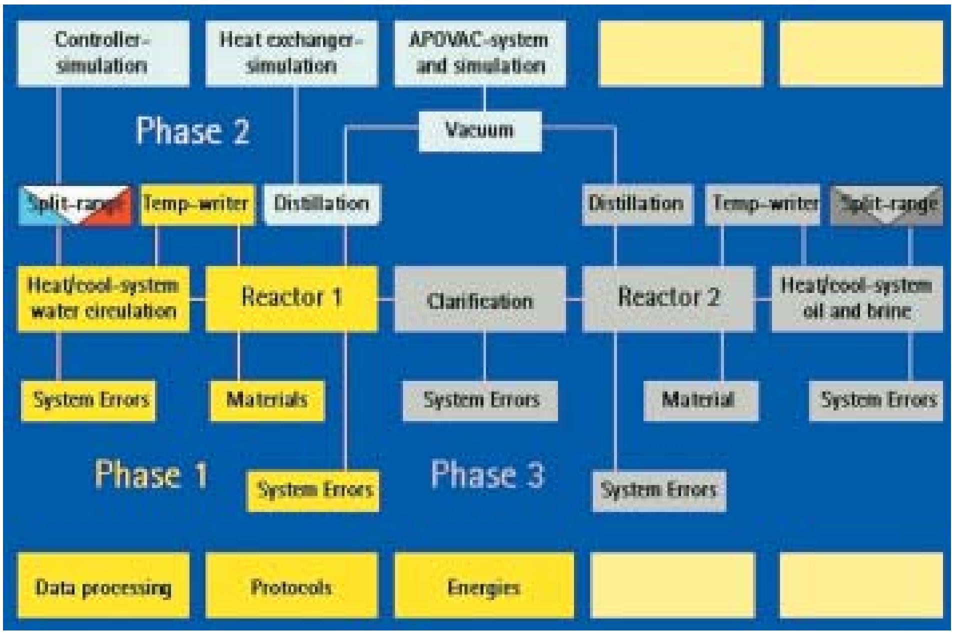

Fig. 14. Block scheme

Our IT-apprentices built the hardware for 15 training-stations and one server including the configuration of the Windows 2000 local area network (Fig. 13).

Planning, technical description and design of the first simulation part was realized by a taskforce of *aprentas,* which was led by Hajo Lehmann.

In order to make it as easy as possible for our apprentices, the use and the visualization of the system is adapted to familiar equipment in our training pilot plant. A multipurpose reactor system to run different basic chemical reactions is already in use (Fig. 14).

The next important step is to extend the layout of the current simulation equipment to operate different kinds of distillation processes. A second reactor with an alternative heating/cooling system and a clarification step between those two reactors is planned. For basic and advanced training we intend to design system details in process automation and control to meet any requirements and technical problems our clients are facing in their daily business.

aprentas can offer to customers a wide and extensive range in new specific training possibilities for employees working in chemical or pharmaceutical production plants.

Training programs and further information available on *www.aprentas.com*/Ausbildung Produktion.