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POSITION PAPER

Process Simulation – Fit for the future?

Position paper of the ProcessNet working Committee Process Simulation, Process Synthesis and Knowledge Processing, 2021

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Introduction

Since its beginnings in the 1970s, process simulation has undergone a considerable development. Today, it is possible to model and simulate very extensive processes or even process networks with complex behaviour of substances accurately in steady-state and dynamic mode. This includes not only conventional chemical processes, but also many special processes, for example from bio- or polymer technology. The coupling of fluid and solid processes can even be realised in one simulation today and the integration of CFD approaches in plant models is also already possible. Due to these diverse possibilities, process simulation has become an established and indispensable tool in the development, design and optimisation of chemical processes.

In the future, process simulation will become even more important as digitalisation in the chemical industry continues to advance. The comprehensive information about existing or possible states of the processes that simulation can provide will flow into a variety of higher-level applications and thus be used by a wider range of users. Flowsheet simulations will thereby develop from a personal tool of the individual engineer for solving specific problems to an integral part of the technology package. This development results in a number of requirements for process simulations. Open interfaces, modularisation and efficient data connections are essential for linking process simulation with other applications. Furthermore, the use of process simulation in higher-level applications implicates additional demands such as higher accuracy, more robust convergence and shorter computing times. New solutions for these demands are foreseeable with advancing digitalisation, as it provides efficient access to comprehensive information as well as very flexible data-based modelling options. These options enable the integration of real data into simulations and the completion of physical models with data-driven approaches.

In view of the upcoming change of process simulation towards an integral part of a networked environment, the question arises whether the methods and tools for process simulation existing today already meet the future requirements or which developments are necessary. This position paper addresses this question from the perspective of users in the German chemical industry who are represented in the ProcessNet working committee “Process Simulation, Process Synthesis and Knowledge Processing”. It represents a common understanding of the committee members and is addressed to developers and users of simulation software from industry, universities and development institutes. The position paper describes the current situation and presents future challenges with possible solutions for a future simulation landscape as part of a networked environment.

Status quo of Process Simulation

In the chemical industry, process simulations support the entire life cycle of a chemical process from development, design and construction to optimisation of operation. In order to provide this support efficiently, the process models for the individual phases must be developed as seamlessly as possible along the life cycle. This is done in the companies by using extensive programme systems, mostly from one manufacturer. Companies with their own in-house simulators have also integrated these into their workflows. The comprehensive programme systems have been developed over the last decades by a few manufacturers on a long-term basis. They cover stationary and dynamic simulations for continuous and batch plants as well as many special applications. Even though these systems are very diverse, there is still no simulation environment that can represent all aspects of the life cycle of a process sufficiently well. The use of the programme systems therefore does not necessarily represent an optimal solution for the process industry. Rather, the process industry is also interested in open, modular solutions for the individual aspects of the life cycle. In addition to the advantage of being able to use the optimal simulation tool for each aspect, the open concept would also reduce the strong dependence on the providers of the programme systems.

Today’s commercial process simulators have been developed as stand-alone tools and are currently largely designed as closed, independent systems. They include all necessary functionalities for a process simulation. This includes a module for calculating the physical properties and reactions, the models for the process units as well as numerical solvers and optimisers. In addition to these functionalities, the process simulation requires the structural information of the process, i.e. the connections between the individual process units, which are usually entered via a flow diagram. Finally, process specifications are necessary to describe the mode of operation. The graphic shows the independent overall system for a conventional process simulation.

The use of a comprehensive uniform programme system for process simulation has been successfully established in most companies so far. A major reason for this is the standardisation, reduction and maintenance of interfaces which connect process simulations with the companies’ systems. The connections range from design data transfer for engineering to process models for real-time optimisation in operation. Over time, numerous interfaces have been created in the companies, which are often specially adapted to the simulation software used in each case. This has enabled the companies to establish very efficient workflows, although this is accompanied by a strong dependence on the simulation software used in each case. Due to the strong integration into the infrastructure, a change of simulation software in the companies is therefore only possible in the long term with a great deal of effort.

The independency of the individual commercial software packages hinders the exchange of simulation models between different process simulators. Currently, no universal flowsheet language exists for the process structure that would enable a simple exchange of models between different simulators or an automatic generation of flowsheet simulations. An even greater challenge than the transfer of the process structure, however, is the transfer of the calculation models for physical properties and reactions. In the various process simulators, different physical properties and reaction models are available for selection, which only draw on internal parameter databases of the simulators. Physical Properties and reaction models are therefore very deeply integrated into the process simulators and accordingly difficult to migrate. On the other hand, the created models represent a very high value for the companies, as a lot of effort and sensitive know-how goes into their creation. The exchange of simulation models between different process simulators is certainly important for industrial companies, in the case of development co-operations, company mergers, process licensing or the transfer of a process simulation to a special software such as operator training systems. Currently, the transfer of an existing process or unit model to a new software environment is only possible with a great deal of manual effort.

The interoperability of process simulations is far from sufficiently developed. For example, the integration of external models into a process simulation often still requires a lot of effort, as process simulators mostly use individual internal interfaces between their modules. Although most process simulators provide interfaces for the integration of external modules, these interfaces are usually simulator-specific. Therefore, the use of ready-made specialised models from third party manufacturers, licensors or from university research is very limited in commercial process simulators. The connection of process simulations from different manufacturers in higher-level composite simulations is also not easy and quick to realise. At the same time, companies are increasingly trying to exploit new potentials by optimising bigger process networks. The comprehensive use of process models also requires the integration of confidential internal company data sets, for example for cost allocation, alternative capacities or reserves.

CAPE-OPEN is an initiative of users and manufacturers of process simulators with the aim of defining uniform interfaces for the exchange of models. CAPE-OPEN basically offers the possibility of an open software environment with exchangeable modules. Unfortunately, the CAPE-OPEN interfaces are not fully supported by all commercial process simulators. When integrating physical properties models via the CAPE OPEN interface, there are still performance deficits compared to the native calculations of physical properties within the simulators. This noticeably slows down process simulators, since a considerable part of the numerical effort in process simulations is spent on calculating the physical properties.

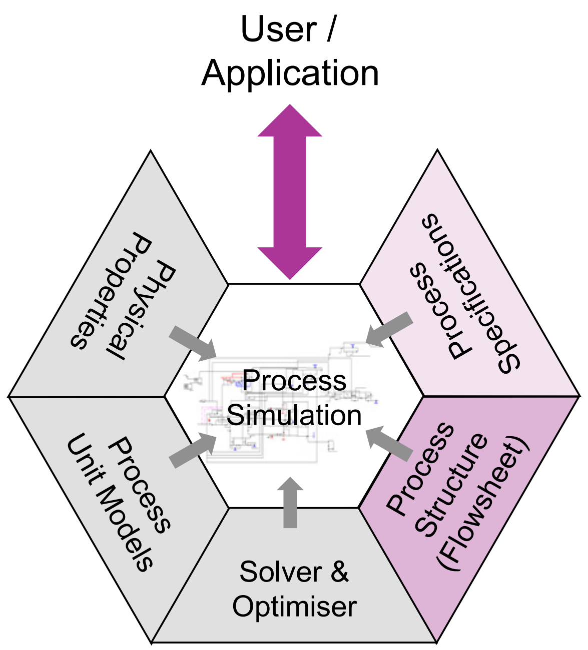

Fig. 1: Overall system of a conventional process simulation

The introduction of technical innovations in the commercial software packages for process simulation is sometimes very delayed, as the manufacturers of the simulation software are naturally limited in their implementation due to the scope of the programme systems and the breadth of the requirements. Individual companies often have little influence on the introduction of new developments in the commercial process simulators. Companies with their own in-house simulators, on the other hand, can implement their ideas much more flexibly, so that these companies have been able to achieve technological advantages in recent years due to the rapid introduction of new approaches that emerged in the environment of digitalisation.

In the individual sections of the process life cycle, simulations are created, extended or modified in the companies by different users in different departments. All this leads to a multitude of process simulations for different aspects that have to be managed and updated. Currently, no commercial provider of process simulators comprehensively supports the documentation, management and updating of process simulations in the process life cycle. Since the problem of updating, reusing and managing is already leading to efficiency losses in the companies, there is a demand for a suitable model management system. A model management system should be able to manage several simulation environments, also with regard to future modular, open systems.

The adaptation of equipment models to specific requirements of the process life cycle with regard to model assumptions, conservation variables, boundary conditions or phenomenological correlations is in many cases only possible to a very limited extent. On the one hand, parts of the equipment model may not be sufficiently documented, or software interfaces for application-specific additions may not be available. This leads to application- or operator-specific additions being included at process model level, which increase the complexity of the flowsheet, and are often not sufficiently documented.

In the future, the simulation-based support for the entire process life cycle will require that dynamic simulation will become more important in addition to steady-state process simulation. However, when moving from a stationary to a dynamic process model, a wide range of model assumptions must be made, for which a user receives insufficient support in the currently available process simulators. With the creation of a dynamic process model, the modelling process therefore often begins anew.

Future Challenges

Originally, process simulators were developed as stand-alone engineering tools to support process development. Today, process simulation has a much broader application, as simulation models can now describe the behaviour of chemical processes in detail in different facets. Process simulations support decisions in planning and operation and also serve to monitor, control and optimise processes. In the future, the use of process simulation will increase even further, as the chemical industry is working intensively on the development of digital twins for its value chains. In the digital twin, process simulation plays a central role as a behavioural model of the chemical process. In this transition, flowsheet simulations are increasingly evolving from a personal tool for the individual engineer to solve specific problems to an integral part of the technology package with an expanded user group. This development results in some consequences for the process simulation.

- » Modularisation of the process simulators for better integration into the technology package
- » Open, standardised interfaces to other programme packages
- » Networking with other applications and expanding the user group
- » Data connection

In the future, process simulations will also benefit from data-driven methods. Possible applications are the identification of interesting operating points in large data sets, the creation of efficiently executable surrogate models and the complementation of physically based models with model extensions based on experimental data. The upcoming challenges for process simulation are discussed in the following.

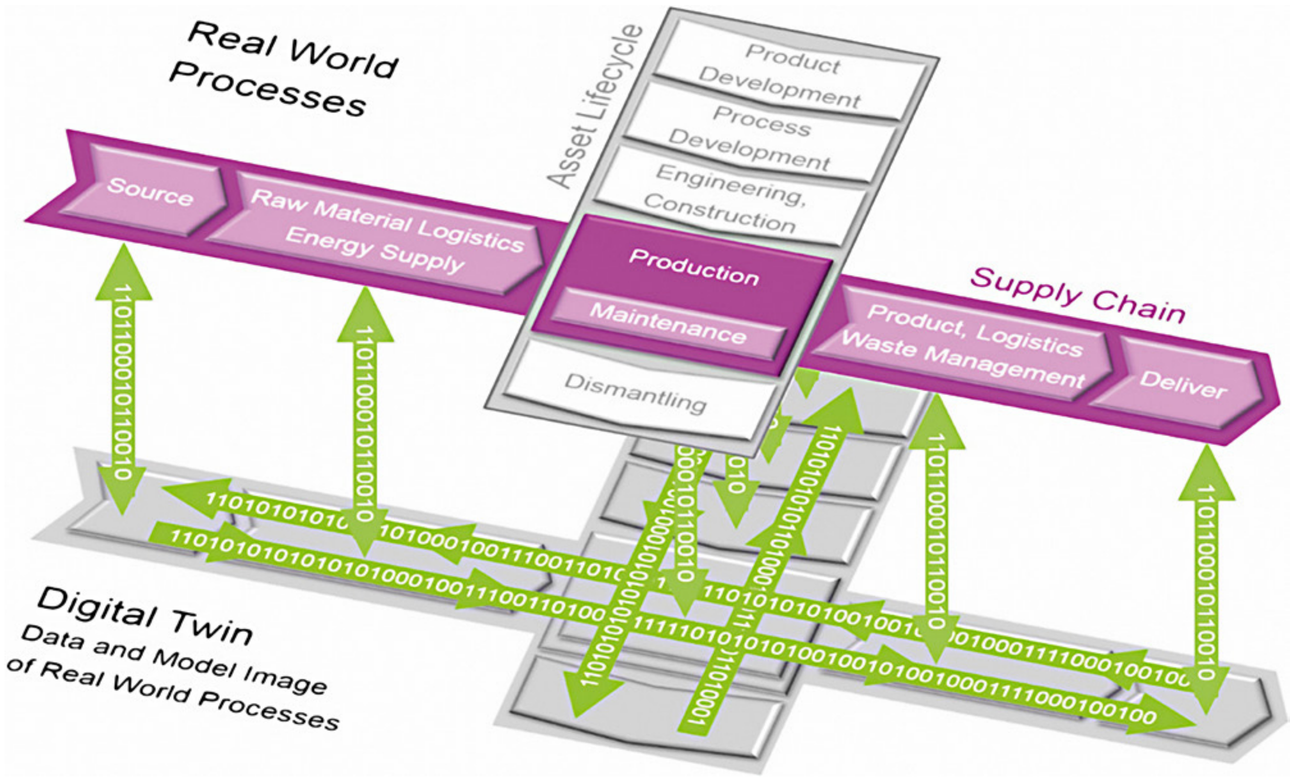

Fig. 2: Digital twin of value chains in the chemical industry. Process simulation is a central component as a behavioural model for the process

Connection to process life cycle data – timeliness and sustainability

One goal of digitalisation in the chemical industry is the fast and structured access to data from the process life cycle. This means that structural information about the current status of the plants will be continuously updated and efficiently available in the future. This includes the interconnection of the individual process units as well as the specification of the equipment currently in use. In process simulators, this information is now permanently entered and must be manually adapted to the current status. It is therefore obvious to link the process simulation with the available data from the process life cycle in the future and thus create the possibility to automatically update the structure of the simulation models. This would be an important step towards solving the long-standing problem of keeping simulation models up-to-date in the long term, as mentioned above. In addition, the workflows in process development and optimisation could become considerably more efficient. For example, the information about a new pipeline or a replaced heat exchanger would flow into the CAE data system directly after the work has been carried out and could then also be immediately available in the process simulation. On the other hand, results from simulation studies could also flow directly into the CAE systems. However, it should be emphasised here that linking the process life cycle data with the process simulation is only a first step, because on the process simulation side, automatic updating can result in new challenges such as the modelling of newly inserted process parts or even the convergence of the automatically updated process simulation.

The benefit of a closer and sustainable connection between process simulation and CAE systems, in which the workflows of the process life cycle are mapped, has already been recognised by software manufacturers. As a consequence, close cooperation between manufacturers of CAE systems and simulation software has recently emerged, which in some cases has even led to takeovers. Companies that use simulation software and CAE systems from two cooperating partners will benefit greatly from this development, but at the same time increase their dependence on the partners. Overall, however, an open, system-independent connection between process simulation and CAE system would be advantageous, as this would allow any systems to be freely combined with each other.

From the design to the operation of a process, there are various application areas for process simulations, these include

- » conceptual process design (including short-cut based),
- » process and equipment design,
- » offline optimisation and bottleneck analyses,
- » virtual commissioning,
- » training simulator and
- » operation, real-time optimisation, condition monitoring, predictive maintenance.

There are currently noticeable breaks between these application areas, where knowledge in the form of models is partly lost. At the same time, the availability of laboratory and process data increases in the course of development. It would therefore be desirable to achieve more model and data consistency in the future. This is also a goal of digitalisation.

It will probably not be possible to achieve consistency with a single simulation tool as it is known today. For example, the model developer has very different requirements for a simulation model than an operations team, and the same applies to the use of data. The challenge for a future simulation and data environment is to improve the consistency of data and models, and at the same time to provide the "right", adapted man-machine interfaces (machine = computer).

This consideration must be taken into account in an intelligent software architecture. This is about interfaces, but also about good development environments for teams. Central model management systems ("model repositories") equipped with intelligence for user requirements and consistency in the software architecture can be an approach here.

Incorporating data-driven models – accuracy and prediction capability

Process simulators are currently based on rigorous and empirical models for the physical and chemical properties as well as for the process units. Since, on the one hand, not all effects in a real process can be captured in a process simulation and, on the other hand, the rigorous and empirical models used only approximate reality, deviations between simulation results and real process data always occur. Process data reflects reality and is becoming much more easily and comprehensively accessible in the context of digitalisation. In addition, data-driven models are available today that can be flexibly adapted to large multidimensional data sets. This adaptation ("machine learning") provides purely data-based models, most of which have no physical-chemical basis and whose extrapolability is therefore very uncertain outside the adapted data range. Even in the adapted domain, sufficiently distributed and reliable data must be available for the adaptation.

In order to increase the accuracy of process simulations, hybrid systems will increasingly emerge in the future, which will have a classic rigorous-empirical model component and a data-driven model component. Concepts must be developed on how to combine the two parts depending on the application. For example, at the beginning of a process development, data-driven models can only support the modelling of the physical properties, while the process modelling remains rigorous due to the lack of data at this early stage of development. In contrast, process simulations for the control and optimisation of existing plants with extensive, available data history for the operating range can include a data-driven model component to describe the real effects more accurately. Overall, the challenge is to combine experience from real process data with rigorous empirical knowledge, depending on the application, to create accurate models that can be extrapolated. Finally, all this has to be incorporated into process simulators in a flexible, clear and user-friendly way.

Currently, data-driven models are not yet part of the standard models of commercial process simulators and must be connected as external software via interfaces. Certainly, an efficient integration of data-driven models is necessary for the execution of process simulations. However, the question remains whether the data-driven models should become part of the process simulators. The process simulators would then also have to provide appropriate tools for training the data-driven models. It would be more flexible to create suitable interfaces and leave the data-driven models together with the training externally. This would also ensure that innovations in the rapidly progressing development of data-driven methods could be incorporated into the process simulation in a timely manner.

The prediction accuracy of data-driven models does not depend solely on the number of data used for fitting but is also significantly determined by the distribution of the data in the application domain. Therefore, methods and tools for sensitivity analysis and design of experiments must be available, which help to determine where which data is necessary in the application domain in order to achieve the highest possible prediction accuracy of the models. Especially for multidimensional problems, it is necessary to find a good balance between the amount of required data and the achievable reliability of the models. During simulation, compliance with the validity range of the data-based model parts must be constantly monitored, as their meaningful ability to extrapolate is not necessarily guaranteed.

Speed, robustness and optimisation

The future use of process simulation in new applications requires high computing speeds and robustness. For example, the use of process simulation in online control applications requires very robust and reliable solutions in the operating range. If, on the other hand, process simulation is to support decisions in planning, numerous fast solutions in an extended parameter range are required. This is especially true for multi-criteria optimisations, which are increasingly used to support decisions. In order to ensure robust and fast simulations, it must be avoided that process simulations search for solutions in physically invalid parameter ranges for an unnecessarily long time For this purpose, methods are to be developed in the future with which the range of valid parameters can be estimated..

Many companies are increasingly creating opportunities for high-performance computing through their own computer clusters or through the use of cloud computing. So far, this development has only made limited use of process simulation. However, based on past experience, it is foreseeable that the increasing computing power will lead to the use of process simulation to solve increasingly complex and extensive problems. Examples of this are

» More extensive and complex flowsheets up to networks with interconnection of individual process simulations

» Increasing modelling depth for physical properties, reactions and process units

» Connection of process simulation to other areas such as CFD, equipment health monitoring, supply chain, etc.

» Optimisations and variants for increasingly complex flowsheets

» Dynamic simulations with more variants and greater modelling depth

To enable this development, process simulations must be able to run on the high-performance computing systems. For the integration of the process simulation into complex higher-level applications, the open interfaces are again a decisive building block.

Today's commercial process simulators use their own integrated equation solvers. These solvers are specified by the manufacturer and are part of the software package.

There is no possibility to use external equation solvers. At the same time, very powerful equation solvers are already available today in widely accessible program libraries, and there is an ongoing evolution. This potential of powerful solution algorithms for non-linear equation systems cannot be fully exploited for process simulation at present. An open concept to decouple the formulation of the physical-chemical relationships and the creation of the system of equations from its solution is not yet offered in commercial process simulators. Approaches to this would be, on the one hand, to provide interfaces for the integration of external equation solvers and, on the other hand, to expose residuals and derivatives of the system of equations for numerical solution algorithms. Such open concepts are successfully applied in research and development. In addition, many companies have the competence to optimise complex simulations in terms of convergence and speed with an open concept.

In general, companies often need innovations and methods from universities and research institutes in their projects. Universities and research institutes should therefore in principle be able to develop solutions for special tasks in simulation, optimization or data processing and to connect them efficiently with commercial process simulators. Suitable interfaces must also be available for this.

For optimisation, commercial process simulators only rely on internal algorithms, although it is in principle possible to connect a process simulation to external optimisers of one's own choice. However, this is complex and associated with performance losses. The external optimiser then carries out a search for the optimum with the help of process simulation calculations, whereby mostly derivative-free methods must be used. Alternative solvers could be used if the system of equations of the process simulation could be exported including the derivatives. Then the optimality conditions could be evaluated directly with efficient procedures. Unfortunately, the commercial process simulators do not yet provide the necessary information to have the freedom to follow this path.

Data-driven models can describe very complex, multi-dimensional relationships well. They can therefore be used as substitute or surrogate models for entire process simulations or parts thereof and provide very fast and robust simulation models. To create surrogate models, simulation calculations in the parameter range of interest are first carried out automatically with conventional process simulations using a suitable exploration strategy. Subsequently, the surrogate models are adapted to the results of the simulations. In principle, real data from operation, pilot plant or laboratory can also be included in the adjustments of the surrogate models, which leads to a hybrid approach. The simulation calculations can be very lengthy due to slow convergence and complex numerics of the original process simulations. Therefore, methods for design of experiments are under development in order to keep the number of variations to be calculated low. An iterative procedure is to be aimed for: Low point density screening is done first. The users then decide which areas of the entire design space should be resolved more finely. Here, the original process simulation should remain unchanged. Overall, when using surrogate models, the computational effort is shifted forward from the actual application to the model adaptation.

Besides speed, the use of surrogate models has even more advantages over the direct use of the original process simulations.

- Significantly reduced convergence problems, e.g. through efficient evaluation or avoidance of discontinuities,
- possibility of global optimisation on the substitute model under certain circumstances (depends on its structure),
- independent of installation and licence for process simulation software or single models,
- no in-depth knowledge required to operate the simulation software,
- open interfaces and
- hybrid approach with integration of external data possible.

By exploiting these advantages of surrogate models, the areas of application for process simulations in planning and development departments as well as in operation will foreseeably expand significantly.

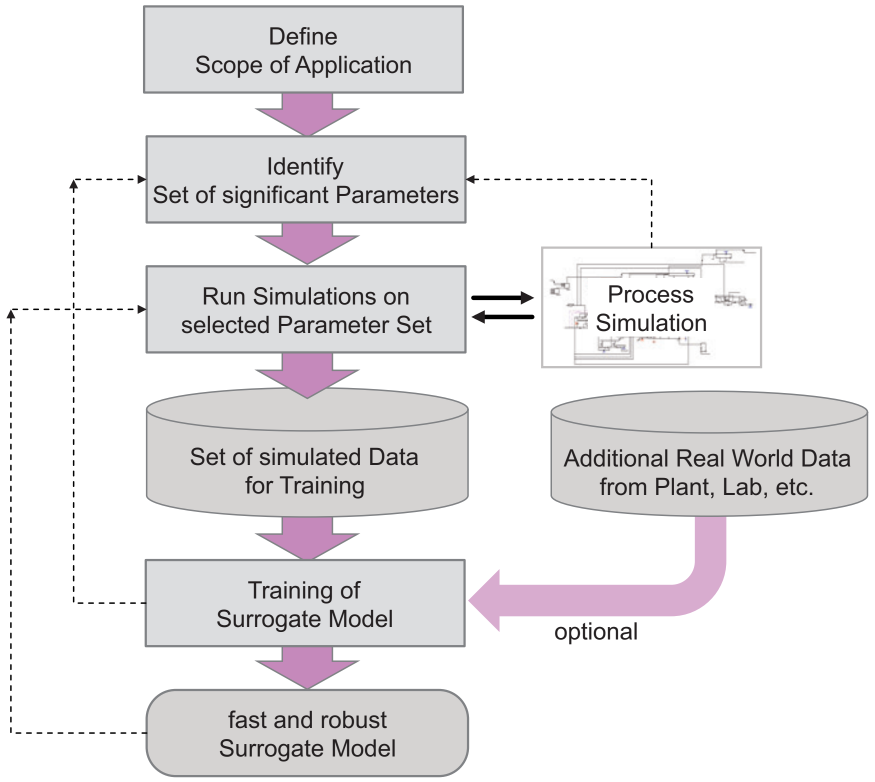

Fig. 3: Procedure for creating a surrogate model based on process simulations with the inclusion of real data from operation and development

More intensive use of process simulation in operation

Process simulations are images of real chemical processes, about whose behaviour they provide data and information. In fact, the operating teams should therefore have direct access to process simulations in order to be able to immediately retrieve information on the operation of the respective process. This can range from monitoring the operation, to case studies, to recommendations for operation through real-time optimisations. Immediate access to process simulations is far from being standard in plants. Besides the costs, the main reasons for this are the maintenance and updating of the simulation models, their accuracy and the operability of the process simulators.

For the maintenance and updating of the simulation models, the connection to the CAE systems as described above is a necessary first step. However, the models for use in operation (for example, training simulators or production optimisers) will differ in part from the models of the process development. Therefore, it is not comprehensively clarified who maintains the models for operation and thus ensures their operation and preservation. This could be done in a model management system, already mentioned above, which is very desirable from the company's point of view. The applications in operation would also be managed in this system.

Access to historical and current operating data from process simulations is no longer a problem today, so that the integration of data-driven models will ensure sufficient accuracy and consistency with reality even for complex processes. Surrogate models can also be used here in the future as sufficiently fast and robust solutions.

For use in operation, dynamic models are often required, the development of which requires a not inconsiderable additional effort. It would be desirable to better support the transition from stationary to dynamic models and simulations so that the knowledge already incorporated in the stationary simulations is used efficiently. In addition, steady-state and dynamic simulations must not "drift apart", the steady-state behaviour must only deviate from each other to a small extent. The direct calculation of a steady state with a dynamic model would be of great advantage here. The development of data-based models of dynamic processes places special demands on the available data, because not only the interesting operating range in the sense of the ranges of process variables must be covered, but also the relevant part of the dynamic behaviour.

The use of process simulations to control, regulate and optimise processes poses a particular challenge, especially if the simulations are not only to provide recommendations for the operating personnel, but are to access the process directly. It must be ensured that the simulations either cover the entire operating range or indicate that they are leaving their range of validity. Especially for data-driven models, suitable test methods must be developed for this requirement. The use of process simulations in Good Manufacturing Practice (GMP) environments is also conceivable. However, appropriate procedures for GMP certification of simulations with the associated computer systems are currently still lacking.

The handling of process simulators is often not designed for use by operating personnel. For use in operation, the handling of process simulators must therefore be appropriately configurable in order to be able to meet all the requirements of the operating personnel. A role concept with corresponding authorisations for the different users would be a solution here. In addition, simple, intuitive operation via a flowsheet should be possible. A very important aspect is also the possibility to easily switch between stationary and dynamic simulation in a process simulator in both directions. This functionality is of course of general interest, but especially for operating teams, it would raise the acceptance of process simulation if steady-state and dynamic investigations could be carried out in one environment.

Physical Properties – Towards a centralised management

The calculation of physical properties is an integral part of all commercial process simulators and comprises a selection of models for the calculation of the physical properties with the associated model parameters. Within the simulators, the models can be combined with each other and the parameters are freely accessible. Those working on the simulations can therefore individually design the calculation of the physical properties, so that in principle each simulation carries its own physical properties model with it. This individuality can require extensive, time-consuming readjustments if process simulations are to be transferred between different software. It is often by far the most time-consuming step in a software change and the biggest hurdle. Another problem lies in the administration of physical properties within companies in this constellation, since in principle the same processes can be calculated with different physical properties. However, physical properties are actually universal and process-independent. The administration of the physical properties' calculation should therefore be taken out of the simulators with the aim of ensuring uniform physical properties calculations for the processes in a company. This also secures the high value of the company's internal physical properties and makes it accessible in a structured manner.

The first step is to limit the calculation of physical properties to the methods that are best suited for the respective processes in the company. For these methods, the associated parameters must be adapted as best as possible, thereafter stored and maintained in a central database.

In the process simulators, the physical properties calculations can now be realised as follows. If the selected calculation methods for the physical properties are available in the process simulators, they can be used there. However, the model parameters must be provided externally from the central parameter database. Within the process simulators, it must be ensured that only the selected calculation methods are available for selection.

Alternatively, the physical properties calculation could be done in an external module with access to the central parameter database. This approach has the advantage that this external module can be used not only in process simulators, but also for other applications in the company. In this way, a consistent calculation of physical properties can be realised throughout the company beyond the process simulation.

Most commercial process simulators have interfaces through which an external calculation of physical properties can be integrated. CAPE-OPEN is such a standardised interface, which is supported by some commercial process simulators. According to previous experience, an external physical properties calculation with connection via interfaces always leads to a loss of performance compared to the native internal calculation. Recent developments in the CAPE-OPEN community aim to increase the efficiency of the interface software.

One way to solving this performance problem would be to create an external physical properties calculation module with a manageable number of selected methods. This module should be made available to the manufacturers of process simulators as source code. Then, the manufacturers could integrate the module directly into their simulator without a loss of performance. A comparable approach was pursued by the IK-CAPE initiative in the 1980s.

Data-driven models can also be applied for modelling physical properties and reactions. AI techniques can be used here to estimate missing physical property data and to increase the accuracy of existing models. However, the challenge is to ensure that basic thermodynamic relationships are fulfilled in order to obtain consistent results. In addition, the adapted models must deliver reliable results in the entire application range. Possible extrapolations are critical here. Even if data-driven physical property models for process simulations are still under development, they must become available in process simulators in the short term.

The modelling of chemical reactions in the process simulation shows many similarities with the modelling of physical properties. The reaction models with their parameters are also deeply integrated in the process simulators, freely configurable and difficult to migrate. An analogous approach can therefore be taken for the management and modelling of chemical reactions.

New aspects for qualification

The transition of process simulation from an independent engineering tool for specific questions to an integral part of the technology package also changes the qualification requirements for developers of process models and simulations. Up to now, engineers and scientists were able to acquire additional knowledge about numerics, computer science and mathematics on the job or on the side, however, the future requirements are more diverse and extensive, so that they have to be imparted in university education. The basics of steady-state and dynamic simulations must be taught during studies, and corresponding tools should be applied in design projects and theses. In addition, integration into the technology package also requires knowledge of data structures, IT architectures, interfaces, programming in modern systems and languages, etc. Effective cooperation in interdisciplinary teams is particularly important here.

The use of data-driven models requires knowledge of the various approaches that can be used, their possibilities and limitations. Here, practical experience in student research projects or internships is important in order to gain a well-founded reference to the possibilities and limits of data-driven modelling. In companies, process simulations are becoming increasingly extensive and complex. Complex simulations should therefore also be available for training to give an impression of the effort that is required here. One example would be real-time simulators of larger plants for studies of dynamic behaviour.

With all the innovations with the additional requirements, it should not be forgotten that the goal is to model real processes, for which the developer of a simulation must have a good understanding of the process. A solid basic education in the classical engineering subjects therefore remains essential and must not be restricted. Only this sound basic knowledge enables the developer of process simulations to understand and evaluate the simulation results.

Summary – A Concept for the Process Simulation 2025+

Figure 4 shows the structure of a process simulation with the extensions resulting from future requirements. The concept of the closed, independent process simulation environment from Figure 1 will then increasingly change into an open system of flexible components that is integrated into a digital infrastructure. The most important extensions are summarised here once again:

» Transparent and widely accepted open interfaces between software components

» Connection to the process life cycle data (asset life cycle) for automatic updating of the process structure

» Connection to operating data for use of simulations in parallel to the current process

» Decoupling of physical properties and process simulation for central management of consistent physical properties calculation in different applications

» Integration of data-based models with training on historical operating data

» Switching between dynamic and steady-state simulations and ensuring consistency between the two

» Opening for external process models to integrate specialised models

» Opening for external equation solvers and optimisers to improve computational speed and robustness

» Provision of the process model in implicit (o=f(x,u) or explicit (x=f(u)) form with derivations for external mathematical solution algorithms.

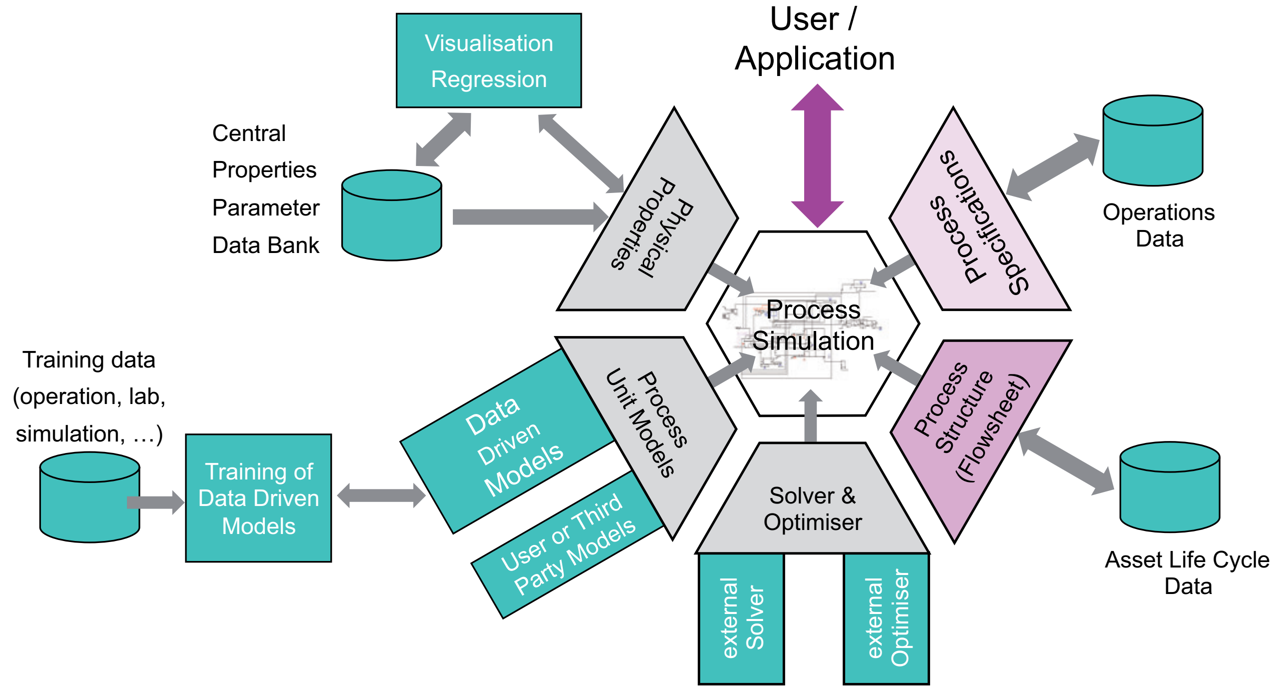

Fig. 4: Structure of the future process simulation (Surrogate model of the overall simulation not shown, see Fig. 3)

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