Where sensation and mathematics meet

Process and plant designers are agreed: Simulation tools have revolutionized their work. Has an el dorado of unlimited possibilities opened itself up to process engineers? Or are they still coming up against limitations today?

GABLEA RIEZSA

Whether for designing a new chemical plant or optimizing an existing one, simulation tools are the method of choice. Starting from thermodynamic process simulation, through dimensioning of equipment, analysis of materials flows and cost analysis, as well as availability simulation through to depicting flows of raw materials and energy (bounding simulations), they provide the designers with their results. But there is a caveat: "Even where simulations are used, we cannot dispense with experiments entirely. But it does mean that fewer tests are needed, in order to verify the simulation. If we didn't have these simulation results, we would have to investigate everything through experiments," says Ingrid Lom- Rieg, Head of Simulation Engineering at Degussa Evonik, in describing the benefits it offers.

Very complex systems and interrelations which cannot always be understood intuitively can be depicted using mathematical solutions. It sounds very easy, but it isn't the case most of the time: "A particularly critical aspect is the application of thermodynamic models which do not fit with the system of raw materials, which provide misleading results," explains Axel Pott, Head of the Conceptual Process Engineering Unit at BASF. A simulation is only as good as the operator and the input data. "Garbage in, garbage out," is the succinct summary from Pott.

Badly-adjusted thermodynamics cause major damage. And a lot of work can be wasted effort if phase equilibria, descriptions of enthalpy and transport data, such as density, thermal capacities, viscosity and conductivity are not correct. "Especially when it comes to the simultaneous description of the reaction and of the transfer of materials and heat, many tools are stretched to their limits. The user needs sound training and experience to be able to identify the traps," comments Konrad Trimbosch, Simulations Expert at Bayer Technology Services. "The training simulator allows us to train for very rare plant conditions, without risk."

Christine Mohr, Departmental Manager Advanced Manufacturing Solutions, Bayer Technology Services

Ideas, born from the simulation, always need to be subjected to a critical examination, as far as possible in a larger-scale team. Discussion with all those involved in the project to validate the results of the model is essential; the expert knowledge of experienced colleagues is much in demand. Even if the planning tool which is simulation is a vital part of the day-to-day work of an engineer nowadays, it requires sensitive and flexible heads to achieve the maximum benefit.

A particularly critical aspect is the application of thermodynamic models which do not fit with the system of raw materials.*

Dr. Axel Pott, Head of the Conceptual Process Engineering Unit at BASF

The author is a freelance journalist at PROCESS.
responsible handling. The simple ease of use, the pleasing graphical user interface and many small and hidden opportunities to make adjustments can seduce inexperienced designers especially to work with the tool almost without thinking. Especially on complex component systems, this can produce false results. "If the operator simply clicks on materials data without thinking about a wide range of new compounds being formed, the simulation outcome will appear highly untrustworthy. For in that case the operator has incorrect materials data descriptions, and the equipment is not dimensioned sufficiently, the separation of components is not possible and the necessary product purity is not achieved," warns Luen-Ring, it is for this reason that younger colleagues work together with older and experienced operators. Furthermore, the computer is not intended to eliminate the need for experiments. It is the collaboration between simulation specialists and experimentalists that produces new initiatives and ideas, ultimately leading to the desired end — optimal plant design.

Surprising results

Now and again, however, the "simulation boffins" hit on a real discovery, precisely because of an error in handling the software. When spraying a smaller existing plant to a larger one and seeking to optimize it, Polt experienced just such a typical input error on his first project. He inadvertently set the hot stream flow to a large vaporization unit to zero. "The result of the simulation was so interesting that we looked at the separation in closer detail. We achieved the specifications practically without any hot steam. This developed into a new process variation with a significant saving on energy."

Cause and effect can be shown in the simulation transparently and quickly. The designers play through a number of scenarios, almost like a video game, providing the team of experts with a sound basis for discussion of the process to be designed. Each person has to take a more global view, looking beyond their particular section of the simulation, in order to avoid misunderstandings and faulty interpretations during the exchange with colleagues.

However helpful software tools are in the design and optimization of chemical plants, now and again they come up against their limits. Traditionally, simulation has become established in the area of fluid process engineering and energy management systems. Beyond that, today's software landscape has a number of missing pieces, according to Treybenbeck: "We lack tools for routine description of complex equipment, in which very fast reactions take place in a multi-phase environment. In some cases, these are played out at the micro level and call for simultaneous description of the flow field and concentration distribution. We are only now seeking the most serious efforts at tackling this."

Growing areas lie in solids simulation and in the simulation of bio-processes. If the findings in terms of the reaction kinetics and materials conversion are deficient, then simulation on the basis of physical models are not suitable. In these instances, assistance is to be gained from empirical, data-driven models on the basis of neuronal networks or hybrid models.

Special conditions

The Chemical Process Industry (CPI) is making use of the achievements of simulation not just in plant design, but also in training plant operators. By connecting a dynamic plant model to the simulator — or even the actual — process control system, they are faced with the same view as is provided by the future measuring station. Unusual situations and special modes of operation can be practiced and visited by staff, without risk. Christine Maul, Departmental Manager for Advanced Manufacturing Solutions, Bayer Technology Services, explains: "In the training simulator you can repeatedly train for highly unusual plant conditions which make high demands of operating staff, without risk. The training allows people to operate the virtual plant to its physical limits and to see how it behaves.

Conclusion: Simulation tools are an essential part of today's CPI. But experienced users know that it is only the plausibility checks, the team exchange of views and simultaneously the experiment which make the software into a practicable tool for planning and optimization.