PROCESS SIMULATION: PAST AND FUTURE

Improvements in computing speed and coding languages have made previously impossible calculations possible. **Jeff Weinfeld, Simon A. Weiland and Ralph H. Weiland, Optimized Gas Treating Inc., USA,** explain how the industry could benefit from embracing these improvements.

Process simulation only became possible with the advent of digital computers. Prior to that, process calculations were almost invariably graphical, with the actual calculations being made by slide rule (see Figure 1). These limitations had their benefits, however. They led to some remarkable simplifications to concepts in stagewise separations, for example, and to how such calculations can be made graphically (c.f., McCabe & Thiele[1], Ponchon[2], Savarit[3], and others).

Figure 2 shows how developments in simulation have paralleled advances in computing. In the mid-1950s, the FORTRAN language was developed and became broadly available, and by the end of the 1950s several oil companies had developed rudimentary process simulators. Of course, all were mainframe-based and extremely user-unfriendly because, although very powerful for numerical calculation, FORTRAN is not well suited for input/output, i.e., graphical user interfaces (GUIs). It was not until the 1980s that desktop computers and personal computers (PCs) were introduced, and user-friendliness became a hallmark of simulation tools. An immediately apparent disadvantage of PCs, however, was their limited memory and the need to squeeze all of the code and data into 640 KB of memory (unless the time taken to swap code and data in and out of memory was acceptable).

An unfortunate fact about simulation tools is that they have tended to apply greater computing power to what are still somewhat antiquated unit operations models, in particular making ideal stage calculations ever faster but without improvements to the underlying engineering science of the separations models, per se. This has left most unit operations models with no more predictive capability than they ever had. Perhaps the

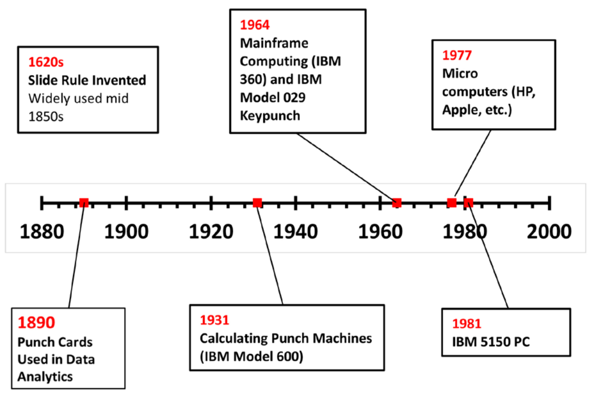

Figure 1. Computers only entered mainstream computation in the last 60 years.

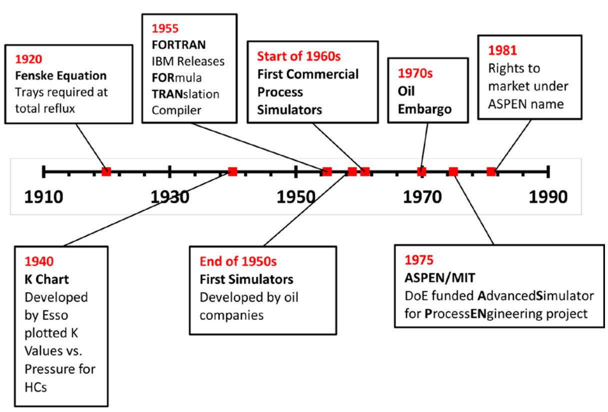

Figure 2. Advances in simulation have almost exactly paralleled advances in computing.

most significant gain from faster computation is the ability to use more complex, increasingly accurate thermodynamics – which is certainly a valuable achievement in its own right. However, unless improved thermodynamics is complemented and accompanied by better unit models, simulations will forever remain correlative rather than predictive.

There have been significant improvements in computing power and programming languages over the last several decades, Computers have progressed far beyond the power and ability needed to make traditional models faster to compute; they now allow us to build such realistic models that simulations can be routinely run with precision and reliability that sometimes challenges our ability to measure the important process parameters. Ideal stages, material balances, and complex thermodynamics no longer define state-of-the-art simulations. Detailed models of the actual transport processes taking place in many unit operations are well within the realm of present-day computing power, but for the most part they remain largely ignored and unexplored. In other words, there are numerous areas where simulation could be used to better advantage than it currently is. This requires development of more detailed, realistic models for the underlying transport processes, as they pertain to commercial-scale equipment.

Digital twins

The concept of a digital twin has attracted a lot of attention recently. However, there are identical twins and fraternal twins, and the ability to pair a digital image with a real operating plant requires as much realism in the computational twin that comprises the simulation. Of course, how much realism is necessary depends on one's expectations from the exercise. At the very least, the digital twin of a unit operation has to be much more than computer code that purports to represent the operation itself; it has to reflect all of the nuances of the operation that matter to its performance, and that allow for it to be designed and operated with confidence and full understanding. Ideal stage models of distillation columns, especially for chemicals, do not meet this requirement, and nor do catalytic reactor models that ignore the effect of pore diffusion, or divided wall column models that fail to treat separations on both sides of the dividing wall(s) as mass transfer rate-controlled processes.

The simulation of a process tends to be viewed as an isolated entity. However, automated unit monitoring introduces the digital twin to the real world of remote control, automation and control without human intervention. The latter is especially important in hazardous processes such as sulfuric acid manufacture.

An example of a product that has already introduced the digital twin to the real world is OGT|ProBot®, which is an excel add-in developed to monitor operating gas treating units and sulfur plants in considerable detail. The OGT|ProBot is already performing unit monitoring tasks in several refineries by acting as the central element in a system that periodically and automatically takes data from a distributed control system (DCS), data historian, or computer control system; launches and runs a high-fidelity computer simulation; then compares results with key plant measurements. Oddities and discrepancies are noted and reported, and then corrective measures are offered, along with alerts about impending equipment failures and future problems being as a result of poor operating conditions – even ones that are hidden and unknown, and that are revealed only by the simulation itself.

Unit monitoring becomes an integral part of the way in which engineers and operators interact with the plant. Automated unit monitoring allows for better maintenance of the integrity of equipment, as well as greatly improved safety performance. This approach depends on accurate predictive models for the process equipment and its operation, and allows operators to pay more attention to process improvements and less to maintaining operations. Additionally, high-fidelity models will almost invariably suggest process improvements.

Cost of simulation

Developing a general-purpose process simulator is a huge and expensive undertaking, if only because of the need for a wide range of thermodynamic models and the corresponding property data for a plethora of chemical systems. Maintaining a general-purpose simulator is an equally arduous undertaking. One of the results is that subscriptions to process simulators tend to become rather expensive. These activities do not leave a lot of room for developing new functionalities and new models for all of the innovative process developments that occur in a year, and for which engineers would like to have accurate models. Furthermore, if one simulator provides models for one specialised process, and another provides models for others, one is faced with paying for subscriptions for multiple simulators. Subsequently, the cost of simulation starts to escalate and become prohibitive. However, there is an alternative, much less expensive solution.

A recent advance in simulation is the development of a protocol that allows multiple software packages to run together without the manual transfer of data from one to the other and with each using its own most-appropriate thermodynamic and properties models. This provides the opportunity to develop a highly-detailed specialised model of great accuracy for a specialised piece of equipment or a specialised set of processing steps that can be connected to the general-purpose simulator via a protocol called CAPE-OPEN.

The specialised software is described as a process modelling component (PMC), also known as a plug. The general-purpose simulator is the central driver (called the process modelling environment [PME], or a socket) which is also protocol-compliant. The CAPE-OPEN standard enables the PMC to be used within the PME without writing any code whatsoever to actually connect the two together. The standard specifies the interface that connects the PMC into the PME. CAPE-OPEN compliant software obeys the rules and protocols established by CO-LaN. Although there are exceptions, most general-purpose simulators comply with version 1.1 of the CAPE-OPEN standards. The version 1.1 standards have much greater flexibility than version 1.0. Also, version 1.0 of the thermodynamic and physical properties interface specification was deprecated from CO-LaN on 1 January 2018. It is very easy to insert a version 1.1 compliant plug into a version 1.1 compliant socket.

OGT|ProTreat® and OGT|SulphurPro® are both CAPE-OPEN compliant PMCs (plugs). ProTreat and its thermodynamics and properties packages from within KBC Petro-Sim are easy to use. Other compliant software includes Xchanger Suite® |HTRI for detailed heat exchanger calculations, and ChemSep for mass transfer rate-based distillation. All are formulated as plugs, and there are numerous others, many publicly available, with others developed by corporations for their own internal use. CAPE-OPEN is an exciting example of how process simulation has developed, and continues to develop, much greater breadth and depth cost-effectively, allowing process simulation to realise much more of its true potential. The future probably does not lie in more comprehensive general-purpose simulators, but in an increasingly broader range of specialised PMCs.

Conclusion

At present, most process simulation is carried out on PCs and desktop computers using software with friendly graphic user interfaces, huge amounts of memory, and fast multithreaded central processing units (CPUs). However, the types of simulation problems that are being solved in the chemical industry, and the unit operations models being applied, unfortunately have not changed substantially. We are still solving the same problems using the same methods – just faster, and to some extent bigger problems.

Two directions that might be taken that will make better use of modern computing and make it more cost-effective have been suggested in this article. One is the approach of CAPE-OPEN to greatly expand the range of detailed high-fidelity models available at quite a modest cost. The other is the use of digital twins, but in the environment of unit monitoring for improved equipment reliability and providing safer process operations. This, too, depends on developing finely detailed models at an affordable cost rather than yet another expensive, general-purpose simulator. Process simulation has a positive future and much room to grow, but greater care needs to be taken to ensure the greatest possible return for the computing dollar.

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