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CAPE-OPEN – What It Does and Why It Matters

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.

A single, truly general-purpose simulator continues to elude us, perhaps because the chemical industry is so extremely broad and encompasses so many diverse disciplines and application areas. Industrial products range from cosmetics to pharmaceuticals, plastics, fibers, paint, pigments and metals to mention only a few. A single simulator is unlikely to meet all the needs of a large commercial enterprise, and subscriptions to multiple process simulators tend to become rather expensive. The activities needed to maintain even a modcum of generality 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. Consequently, the cost of simulation starts to escalate and to become prohibitive. However, there is an alternative, much less expensive solution.

A modern advancement in process simulation is the development of a standard that allows seamless interoperability of process simulators 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 standards specification called CAPE-OPEN. Here, CAPE stands for Computer-Aided Process Engineering. The CAPE-OPEN interface standards is developed and maintained by a non-profit organization called CO-LaN[1].

Structurally and conceptually, CAPE-OPEN is designed to allow the general simulation environment to act as a socket and the specialised software to act as a plug, in a close parallel with the plugs and sockets common in home wiring and electrical circuits. The specialised software is described as a process modelling component (PMC). The general-purpose simulator is the central driver (called the process modelling environment [PME], or a socket). The CAPE-OPEN standard enables the PMC to be used within the PME without writing code to actually connect the two together structurally.

The OGT|ProTreat® and OGT|SulphurPro® programs are both CAPE-OPEN compliant PMCs that can be used as unit operations and/or as thermodynamic servers by other PMEs. ProTreat unit operations and properties packages are easy to use from within KBC Petro-Sim, for example, and many other simulators, as well. Other compliant PMCs includes Xchanger Suite®|HTRI for detailed heat exchanger calculations, and ChemSep for mass transfer rate-based distillation. A number of large simulators are known to be CAPE-OPEN compliant, and there are a number of compliant PMCs, many publicly available, with some developed by corporations for their own internal use. CAPE-OPEN is an exciting example of how process modeling has developed[2] (and continues to develop) much greater breadth and depth cost-effectively, allowing process simulation to realise much more of

[1] Details can be found at https://www.colan.org/

[2] https://www.colan.org/techpapers/cape-open-review-in-chemie-in-genieur-technik/

its true potential.

The future of simulation probably does not lie in more comprehensive general-purpose simulators, but in an increasingly broader range of specialised PMCs. It makes sense to make available to an existing (CAPE-OPEN compliant) PME, one or more modules containing models for specialized unit operations or specialised thermodynamics. This avoids having to provide yet another PME that wraps around the module and allows it to run.

To construct software of any size, modules are built using DLLs. A DLL is essentially a precompiled set of procedures that is linked into a computer program at run time. To use a DLL, one must know the input and output variables (parameter list and any global memory storage structures) that are fed into and out of the procedures. CAPE-OPEN, however, is on a different level.

The purpose of CAPE-OPEN is not to **build** modules. Rather, it is a protocol that provides a standard interface specification whose use permits one to connect independent process simulators without knowing any details about how each one is built. Typical use of any 3rd party module requires knowledge of inputs and outputs; whereas, CAPE-OPEN modules provide these in a structured and standardized manner. Beyond the code needed to make the PMC and PME standard-compliant, CAPE-OPEN completely eliminates the need for writing ad-hoc code to connect a PMC with a PME. This allows a simulation engineer to build highly complex and composite process models with minimal effort in establishing connectivity between a variety of programs.

Conclusion

At present, most process simulation is carried out on PCs and desktop computers using software with friendly GUIs, 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 really changed substantially. We are still solving the same problems using the same methods – just somewhat bigger problems, solved faster.

One direction that might be taken that would make better use of modern computing and make it more cost-effective has been discussed, namely, the CAPE-OPEN standard. Its approach greatly expands the range of detailed high-fidelity models available at quite modest cost. Process simulation has a wonderful future and much room to grow, but greater care needs to be taken to ensure the greatest possible return for the computing investment.

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To learn more about this and other aspects of gas treating, plan to attend a *ProTreat*® workshop in your region. For details, visit www.protreat.com/seminars.

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Conference Alert: OGT will be a proud exhibitor at the 6th annual SulGas conference in Mumbai, from 31 Jan to 2 Feb 2024. SulGas is a technical conference on Sulphur and Gas Processing with an emphasis on South Asia. OGT and 310i will jointly be presenting a paper titled: ***Kinetics-Based Sulfur Plant Models: Advancing Process Understanding***. The conference is currently accepting delegate registrations and has special rates for women engineers and group participation. Details can be found at www.sulgasconference.com.