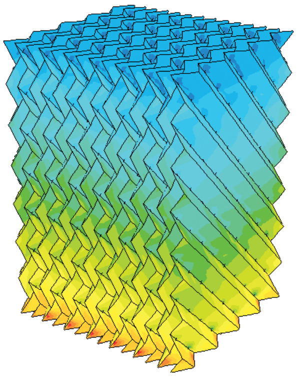
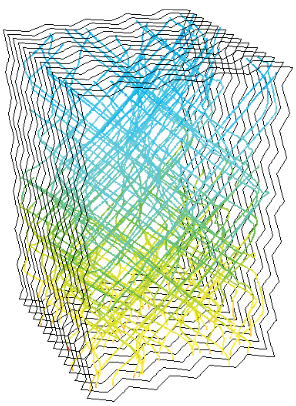
Realistic Distillation Modeling

By Valmor de Almeida, Oak Ridge National Laboratory, Oak Ridge, TN; Rafiqul Khan and David Schowalter, Fluent Inc.



Pressure contours on the surface of structured packing elements in a distillation column



Pathlines, colored by pressure, illustrate the flow through the structured packing elements

Much of the energy required for processing chemicals in the industrialized world is used in distillation columns. Because the multiphase physics and intricate geometry involved in these operations are so complicated, their design remains semi-empirical. CFD modeling offers an opportunity to improve the performance of distillation columns, translating into energy savings, better product purity, and reduced environmental impact. In fact, the US Department of Energy (DOE) estimates that optimization could save trillions of BTUs per year.

The Office of Industrial Technology at DOE has supported efforts undertaken by a team of engineers from ORNL, Fluent, and the Separations Research Program (SRP) at the University of Texas, Austin to modernize the modeling practices in distillation columns and similar chemical processing units. Other partners on the team include Dow Chemical, John Zink Co., Praxair, Sulzer Chemtech, and 3D Imaging and Development Inc. The project has focused on distillation columns that employ a structured packing technique, where packings are fabricated from thin, corrugated metal sheets, and arranged parallel to one another. The approach combines detailed geometry modeling, first-principles simulation, and validation experiments to deliver a realistic simulation tool. A collection of macros, GraSPI (Graphical Structured Packing Interface), has been developed and integrated into GAMBIT and FLUENT. GraSPI coordinates the generation of geometries and meshes for typical commercial structured packing elements and flow simulation.

Simulations to date have involved gas flows through different packing geometries, and comparisons of predicted pressure drop with experiment have identified the minimum mesh size required for a certain level of solution accuracy. GraSPI is currently being extended to handle other packing geometries, such as perforated sheets and cross-stacked cylindrical elements. FLUENT simulations of gas-liquid flows are also being carried out using the VOF model. The ultimate goal is to be able to simulate gas-liquid countercurrent flows through as many packing elements as necessary to produce a realistic model of SRP's pilot packed column. Achievement of this goal will show that accurate, large-scale, first-principles simulation of distillation in structured packed columns is finally at hand. ■