

Optimizing Plant-Scale LDPE Reactors

By Nitin H. Kolhapure* and Rodney O. Fox, Department of Chemical Engineering, Iowa State University, Ames, IA
*Presently at DuPont Engineering Technology, Wilmington, DE

With the ever-increasing availability of high-performance computing tools, CFD is becoming a significant technology, though still not dominant, for reactor design in the chemical process industry. CFD is emerging as a design tool for the development of new processes and optimization of existing ones at a fraction of the cost and time of traditional experimental and pilot-plant approaches. At Iowa State, the ability of CFD to simulate turbulent reacting flows in processes involving fast, mixing-sensitive reactions has been investigated. These flows are characterized by interactions between large and small chemical and mixing time scales that play a significant role in determining reactant consumption (yield), product quality (selectivity), and reactor stability. Traditional reactor models based on idealized flow assume perfect micromixing and fail to account for such interactions.

To improve upon these models, a comprehensive CFD algorithm that links FLUENT with a sub-grid-scale multi-environment micromixing (MEM) model and detailed low-density polyethylene (LDPE) chemistry has been developed for plant-scale tubular reactors. In LDPE reactors, a small amount of initiator is injected into a preheated monomer flow to start a complex series of reactions that produce polymers of varying length (molecular weight). These reactors are extremely sensitive to local mixing

conditions due to stiff and highly exothermic kinetics and hence, they serve as an excellent test case for commercial reactors where control of the reaction conditions and optimization of the reactor performance (i.e., reactor stability, initiator efficiency, polymer molecular weight distribution) are desired.

An interactive interface was created for the project using user-defined functions (UDFs) in FLUENT. C routines for the MEM model and FORTRAN routines for a customized *in-situ* adaptive tabulation (ISAT)¹ algorithm for the LDPE chemistry were compiled and linked to FLUENT. The continuity equation, the $k-\epsilon$ model, the MEM model, and the chemistry were solved sequentially at each grid point in a 2D axisymmetric computational domain. An unsteady coupled implicit solver was chosen to limit the effects of truncation errors on the solution. The UDF interface updated the mixing and chemical source terms at each time step as per the formulation in the MEM model and the ISAT algorithm. The interface also provided an ability to account for the inter-dependence of the kinetic, physical, and thermodynamic properties of the polymer reaction mixture. ISAT enabled the inclusion of a total of 16 species and offered ten-fold computational gains by replacing the conventional direct integration with a less expensive multi-linear interpolation. It proved to be a powerful technique to include chemistry calculations in CFD without restricting the degrees of freedom of the chemical composition vector. More details of the CFD algorithm with the UDF interface and the MEM model can be found elsewhere.^{2,3}

The CFD results demonstrated the capabilities of the algorithm to capture the strong coupling between micromixing and complex chemistry and predict the complete reacting flow information, including species and temperature distributions close to physical reality. The flow information at the micro-scale provided important insights into the occurrence of small-scale temperature fluctuations (hot spots), deterioration of polymer quality, and



The mean mass fractions for initiator (top, 0 to 1.15×10^{-3}), monomer (middle, 0.95 to 1), and temperature (bottom, 250 to 307°C) inside a tubular reactor ($d = 3.8$ cm, $L = 10$ m)



The injection region (0 to 0.2 m) is zoomed in to highlight the non-uniform initiator distribution, which caused a loss of 64% initiator compared to plug-flow conditions

The Berl Combustor Revisited

By Graham M. Goldin, Fluent Inc.

The focus of FLUENT 6.1 gas-phase combustion modeling is to provide affordable, detailed, finite-rate chemistry. With the new models, kinetically controlled processes such as pollutant formation (NO_x , CO, etc.) and flame ignition/extinction can be simulated with high fidelity.

The difficulty in including detailed kinetics is the extreme non-linearity of the chemical mechanism. Large computational times are required to integrate the equation set, and special care is required to properly couple the chemistry with the turbulent flow. For these two reasons, most commercially available chemistry codes are limited to physical dimensions of zero or one.

To overcome the massive computational demands of detailed chemistry simulation in 2D and 3D domains, FLUENT 6.1 incorporates ISAT (*In-Situ Adaptive Tabulation*¹), which can accelerate chemistry calculations up to a thousand-fold. For a chemical mechanism with N species, ISAT builds N-dimensional chemistry tables during the simulation. The expensive kinetic integrations are mitigated by retrieving the appropriate values from the table. ISAT can be used with two turbulence-chemistry interaction models in FLUENT 6.1: the Eddy Dissipation Concept (EDC) model and the PDF Transport model.

To demonstrate the power of ISAT, a FLUENT 6.1 simulation of Sandia's Burner Engineering Research Laboratory (BERL) industrial combustor has been performed using the EDC model. The BERL combustor consists of an annulus with swirling air, into which 24 fuel

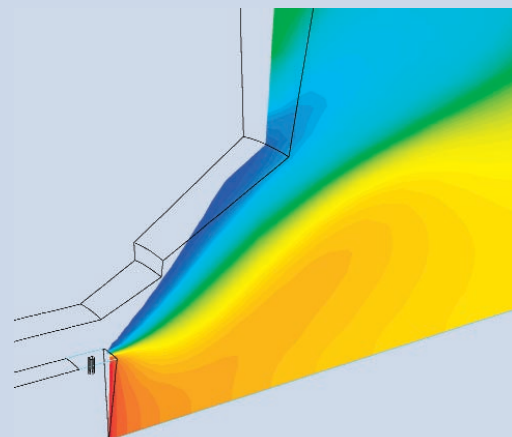
jets inject natural gas. The mixture then enters a quarl, which expands to a hexagonal combustion chamber. Because of its complex physics and ample supply of experimental data, the BERL combustor has served as a benchmark test case for combustion models in FLUENT for many years.

Since the fuel jets in the cross-flow air-stream cannot be accurately modeled in 2D, a 3D sector representing 1/24th of the burner is modeled. The simulation makes use of the realizable k- ϵ turbulence model, and the P1 radiation model. The chemistry is described by a 9 species Augmented Reduced Mechanism (ARM), which was derived from the detailed natural gas mechanism by making steady-state assumptions for certain species.²

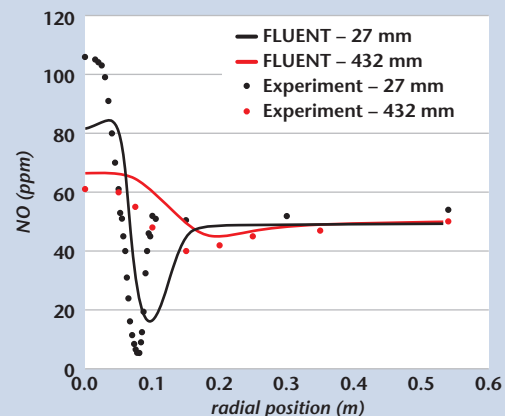
Results for radial NO predictions are in good agreement with experimental measurements at 27mm and 432mm downstream of the quarl, despite the many assumptions made in modeling the turbulence, chemistry, radiation, and their interactions with each other. Radial profiles of temperature and other species concentrations follow the same trends. In addition, ISAT provides a net speed-up of 65 for this case. Without ISAT, a simulation that can be completed overnight would require a month of run-time! ■

references

- 1 Pope S.B., "Computationally Efficient Implementation of Combustion Chemistry Using *In-Situ Adaptive Tabulation*", *Combustion Theory and Modeling*, 1, pp. 41-63, 1997.
- 2 <http://www.et.byu.edu:8080/~tom/Papers/Hemant-WSS96/WSS.html>.



Contours of NO on a center plane near the quarl



Comparison of FLUENT predictions of NO_x with experimental data for radial scans 27mm and 432mm downstream of the quarl

loss of initiator under extreme operating and mixing conditions. The influence of feed temperature, initiator concentration, and degree of premixing on steady-state reactor performance was helpful in making wiser, more well-informed operational decisions. By replacing pilot-plant

tests, CFD offered a low-cost alternative to explore a variety of design options for optimizing initiator consumption while controlling the product quality and reactor safety. Though validation of such a CFD approach against key experimental data remains an integral and essen-

tial part of the design procedure, it opens greater opportunities for the development of safe and efficient chemical processes at reduced costs and time. The study has brought turbulent reacting flow simulation for single-phase finite-rate chemistry closer to realistic chemical process engineering applications. ■

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- 1 Pope S.B., "Computationally efficient implementation of combustion chemistry using *in situ* adaptive tabulation." *Combustion Theory and Modeling*, 1:41-63, 1997.
- 2 Fox R.O., "Computational methods for turbulent reacting flows in the chemical process industry." *Revue de l'Institut Français du Pétrole*, 51:215-243, 1996.
- 3 Kolhapure N.H. and Fox R.O., "CFD in polymer reaction engineering: Combining polymerization chemistry and detailed flow models." *DEHEMA Monogr.*, 137:247-271, 2001.



The effect of micromixing is shown through local temperature fluctuations in the reacting environment (top, 250 to 329°C) and higher polydispersity (molecular weight distribution) (bottom, 0 to 7.15)