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Quantifying the Uncertainty in Multiphase CFD Predictions

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National Energy Technology Laboratory

Frank H. Walk Room (Engineering Lab Annex) ELAB
February 07, 2014 - 03:30 pm

Abstract:

To accelerate the development of technology, such as for example CO 2 capture, decisions about the scale-up of commercial reactors need to be made on the basis of information obtained from pilot scale units 20−100 times smaller. Physics-based computational tools can be used to generate the desired degree of confidence in the scaled up design. Multiphase computational fluid dynamics (CFD) is one such tool that can be used for the design and troubleshooting of fluidized bed reactors, ideal candidates for sorbent-based CO 2 capture. To make design decisions based on multiphase CFD predictions, it is essential that the uncertainty in the predictions be quantified. Recent progress in developing uncertainty quantification methods for multiphase CFD will be presented in this seminar by discussing the two papers Gel et al. (2013) and Storlie et al. (2013).

Gel, A., Li, T., Gopalan, B., Shahnam, M., Syamlal, M., "Validation and Uncertainty Quantification of a Multiphase CFD Model", Industrial & Engineering Chemistry Research, 2013, doi:10.1021/ie303469f.
Storlile, C.B., Lane, W.A., and Ryan, E.M., "Calibration of Computational Models with Categorical Parameters and Correlated Outputs via Bayesian Smoothing Spline ANOVA ANOVA," submitted to the Journal of the American Statistical Association, July 2013.

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Speaker's Bio:

Dr. Syamlal leads the Computational Science and Engineering Focus Area at NE TL, responsible for the development of science-based simulations that span a broad range of scales for accelerating energy technology development and serves as Director of the Carbon Capture Simulation Initiative. He received degrees in chemical engineering: B.Tech from II T (BHU), and MS and PhD from II T, Chicago. He has been the architect of the widely used open-source multiphase CFD code MFIX and led the development of multiscale simulation capabilities linking process and device scales and the C3M chemical kinetics software. He is the recipient of numerous awards such as DOE Secretary's Achievement Honor Award and AIC hE's Fluidization Process Recognition Award.