Other - Enabling Process Innovation Through Computation (EPIC)

Computational Fluid Dynamics in Chemical Reaction Engineering: History, Impact and Potential

Patrick L. Mills, Texas A&M University - Kingsville

Professor and the Frank H. Dotterweich Endowed Chair

Patrick F. Taylor Hall 1106
October 18, 2013 - 02:00 pm

Abstract:

The underlying principles of fluid dynamics and the formulation of the governing equations, such as potential flow, the Euler equations and the Reynolds's Averaged Navier-Stokes equations (RANS) were already well-established in the early 1960's with notable motivation provided by the birth of commercial jet airplanes and space exploration. Advances in computer power and the implementation of new numerical algorithms via robust computer codes provided the basis for the emergence of computational fluid dynamics (CFD) as both an intellectual discipline and as a unique pathway for creating new knowledge on fluid-fluid and fluid-solid interactions in complex engineering systems. During the 1980's and early 1990's, advances in CFD within the aeronautical, aerospace and other technology-driven industries spilled over into chemical reaction engineering, which led to the application of CFD for describing detailed interactions between local transport effects, reaction kinetics and hydrodynamics. Since these initial efforts, the utilization of CFD from a reaction engineering perspective has evolved into a recognized tool for reactor design, analysis and troubleshooting, thereby reducing reliance upon subjective experience and empiricism associated with less fundamental approaches. Despite the increased popularity of CFD, which has been primarily driven by developments in computational hardware and the availability of standardized software packages, several notable challenges must be addressed before it can be used as a tool for direct scale-up from lab reactors to commercial scale units, or for detailed modeling of existing, complex commercial scale-reactors. These challenges create a number of opportunities for continued research and application, especially in emerging technologies where chemical engineers are leading the discovery of new processes for manufacture of advanced materials, fuels, chemicals, and a host of other product-driven industries.

This presentation will provide an overview of the history, impact and potential of CFD in reaction engineering to illustrate the capabilities, limitations and potential of CFD for addressing the challenges associated with advancing existing and emerging process technologies within the realm of advanced materials, fuels, chemicals and other key industries. After providing a historical perspective of the emergence of CFD within reaction engineering, several examples will be presented to the development and application of CFD to reactors involving multiphase contacting as well as complex systems for advanced material-forming processes. Application of CFD to the analysis of microprocessor systems, microreactors and advanced analytical systems will also be described. Selected examples of the current state-of-the art where CFD has been utilized to analyze commercial-scale reactors will also be summarized along with some final thoughts on future developments and needs.

Online viewing: HTTP://CONNECT.LSU.EDU/EPIC-SEMINARS

Speaker's Bio:

Dr. Patrick Mills is the Frank H. Dotterweich Chair and Professor in the Department of Chemical and Natural Gas Engineering at Texas A&M University-Kingsville. Before being appointed to his academic position in January 2006, he was a Senior Research Associate in the DuPont Company's Central Research and Development Department in Wilmington, Delaware. During his 15+ years at DuPont, he used his expertise in reaction kinetics, multiphase reaction engineering, transport phenomena, and experimental systems engineering to impact many technology areas in various DuPont businesses, including Dacron, Nylon, Lycra, White Pigments, Fluoroproducts, and Nonwovens. He was awarded an Engineering Excellence Award from DuPont in 1996 for development of the MARS system, which is an automated catalyst testing productivity device. Prior to joining DuPont, Dr. Mills worked for nearly 10 years at the Monsanto Corporate Research Center in St. Louis and the GE Corporate R&D Center in Schenectady, New York. His research utilized reaction engineering principles for the discovery and development of new molecules and processes in various technologies, such as agricultural and rubber chemicals, detergent hydrophobes, aromatic polycarbonates, and functionalized olefinic polymers. He also served as a Research Associate Professor at Washington University in St. Louis from 1988 to 1990 and was a member of the technology and business team with Dr. John T. Gleaves that commercialized the TAP (Temporal Analysis of Products) reactor system. He also held appointments as Adjunct Professor of Chemical Engineering at the University of Delaware and Washington University in St. Louis where he taught graduate courses in reaction engineering, multiphase reaction engineering, and applied mathematics. Dr. Mills is the author or co-author of over 150 publications in chemical engineering and applied mathematics, has presented more than 150 papers at professional society meetings, and is named co-inventor on several patents. He is a member of the AIChE, Sigma Xi, and the Society for Industrial and Applied Mathematics. He has chaired or co-chaired numerous sessions in reaction engineering at the AIChE annual meetings, served as guest editor for special journal issues and edited volumes, and was elected to serve as Chair of the AIChE Catalysis and Reaction Engineering Division from 2005 to 2006. He also consults in catalytic kinetics, reaction engineering, experimental reaction systems engineering, and process development. Dr. Mills was also a lecturer for the AIChE Continuing Education series in multiphase reaction engineering. He also serves on the editorial board for *Reviews in Chemical Engineering*, *Applied Petrochemical Research*, and is a member of the AIChE Books Publication Committee.

Center for Computation & Technology
2003 Digital Media Center • Telephone: +1 225/578-5890 • Fax: +1 225/578-8957