Imperial College London

UCL

Professor Michael F. Doherty
University of California, Santa Barbara

Crystalline Solids: The Next Frontier in Process Systems Engineering

In the Chair: **Professor Nilay Shah, Director, Centre for Process Systems Engineering, Imperial College London**

Vote of Thanks: **Professor John Perkins**

Abstract: Crystalline organic solids are ubiquitous as either final products or as intermediates in the specialty chemical, pharmaceutical, and home & personal care industries. Virtually all small molecular weight drugs are isolated as crystalline materials, and over 90% of all pharmaceutical products are formulated in particulate, generally crystalline form. Normally, the properties of the crystalline solid (especially polymorph and crystal shape) have a major impact on the functionality of the product as well as the design and operation of the manufacturing process, and in most cases the two cannot considered separately. The current generation of process models for solution crystallization focus on the prediction of particle size distribution for populations of spherical particles. In this modeling environment the growth models are isotropic, and are incapable of predicting the shapes of faceted crystals. Crystal shape, however, is an important material characteristic and there is significant potential value for process models that are capable of simultaneous prediction of crystal size and shape. To be successful in a process simulation environment, shape prediction models must be fast (they will get called hundreds or even thousands of times during a process simulation) and yet faithful to the fundamental chemical physics and interactions governing the development and evolution of crystal shape. To predict crystal shape it is necessary to predict the relative growth rates of the faces which appear on the crystal surface. The rate determining step for the growth of most API crystal faces is surface integration kinetics of solute molecules. Based on this, we have succeeded in developing the first ever ab initio mechanistic model for predicting the relative growth rates of non-centrosymmetric organic molecules of realistic complexity. The key variables on which the model depends are (1) properties of the solid state, such as unit cell, space group, intermolecular potentials, charge distribution, etc, (2) properties of steps and kinks (kink rates that account for non-isotropic behavior, treatment of unstable edges, modified Boltzmann kink distribution), and (3) surface free energy at the crystal-solution interface. The model has been successfully applied to a selection of complex molecular crystals of interest in pharmaceutical and specialty chemical products.

Biography: Michael F. Doherty is Professor of Chemical Engineering and Department Chair at the University of California, Santa Barbara. He received his B.Sc. in Chemical Engineering from Imperial College, University of London in 1973, and his Ph.D. in Chemical Engineering from Trinity College, University of Cambridge in 1977. He taught at the Universities of Minnesota and Massachusetts (where he reached the rank of University Distinguished Professor) before joining the faculty at UC Santa Barbara in 2000. He was a visiting scholar at the University of California, Berkeley for the 1984 calendar year, at the University Institute of Chemical Technology, Bombay, India, January 2005 and January 2006, and at the CNRS Centre de Recherche en Matière Condensée et Nanosciences, Luminy Campus, Marseille, France, 9/2006 – 4/2007. His research interests include process systems engineering with particular emphasis on crystal engineering of organic materials, separation with chemical reaction, and design and synthesis of nonideal separation systems. He is the holder of four patents, has published over 150 technical papers and delivered over 200 invited lectures; he was awarded best paper of the year in 1993 (jointly with M.F. Malone and Z.T. Fidkowski) and again in 2001 (jointly with M. F. Malone and S. B. Gadewar) by the editors of *Computers and Chemical Engineering*. He has received numerous honors and awards for his teaching and research, including the Computing in Chemical Engineering Award of the CAST Division of the AIChE, the Alpha Chi Sigma Award for Chemical Engineering Research of the AIChE (2004), the Clarence G. Gerhold Award of the Separations Division of the AIChE (2004) and the Excellence in Process Development Research Award of the Process Development Division of AIChE (2004). In 2008 he was named one of the "One Hundred Chemical Engineers of the Modern Era" (post 1945) by the American Institute of Chemical Engineers.

Lecture Theatre 1 (Room 250), Department of Chemical Engineering, ACE Extension Building,
South Kensington Campus, Imperial College London SW7 2AZ
Tea and coffee will be served before the lecture from 16.30 in the Common Room (Room 228), Department of Chemical Engineering, Level 2, ACE Extension Building

Thursday 2 December 2010 • 17.30

The Seventeenth Professor Roger W.H. Sargent Lecture

The Professor Roger Sargent Lecture is an annual event the Centre for Process Systems Engineering inaugurated as a tribute to Professor Sargent's vision, leadership, significant technical contributions and to his legacy in the field of Process Systems Engineering.