

# **Chemical Engineering Seminars – TT 2008**

***Week 3: Monday 5 May, 4:15 - 5:15 pm  
Lecture Room 3, Thom Building, Engineering Science***

## **Drinking from a Fire Hose: Modeling Challenges and Opportunities in Molecular Products Design and Manufacturing**

Prof. Venkat Venkatasubramanian

Laboratory for Intelligent Process Systems. School of Chemical Eng., Purdue University

### ***Abstract***

Designing new materials and formulations with desired properties is an important and difficult problem, encompassing a wide variety of products in the specialty chemicals and pharmaceuticals industries. Traditional trial-and-error design approaches are laborious and expensive, and cause delays time-to-market as well as miss some potential solutions. Furthermore, the growing avalanche of high throughput experimentation data has created both an opportunity, and a major modeling and informatics challenge, for material design and discovery. A systematic way to convert the raw data gathered from process analytical technologies (PAT) to information and first-principles knowledge that can be used for real-time decision making is very much lacking. A new paradigm is needed that increases the idea flow, broadens the search horizon, and archives the knowledge from today's successes to accelerate those of tomorrow. All these present considerable challenges, as well as great opportunities, in the area of product design and engineering.

Cyberinfrastructure will play a crucial role in product design, process development and commercial scale manufacturing by streamlining information gathering, data integration, model development, and managing all these for easy and timely access and reuse. In this talk, I will discuss a novel cyberinfrastructure framework called Ontological Discovery Informatics. The foundation of such an infrastructure is the explicitly and formally modeled information, called an Ontology. This framework enables the management of information complexity, accumulation of knowledge, systematic model development, and efficient search for new materials with desired performance characteristics. I will discuss the application of this paradigm for industrial molecular products design problems in the specialty chemical and pharmaceutical industries.

## ***Bio-sketch***

Prof. Venkat Venkatasubramanian is a Professor of Chemical Engineering and a Professor of Industrial and Physical Pharmacy (by courtesy) at Purdue University. He earned his PhD in Chemical Engineering (with a Minor in Theoretical Physics) from Cornell University in 1984, MS in Theoretical Physics from Vanderbilt University in 1979, and BTech in Chemical Engineering from the University of Madras, India, in 1977. Venkat worked as a Research Associate in Artificial Intelligence in the School of Computer Science at Carnegie-Mellon University and taught at Columbia University before joining Purdue in 1988. At Purdue, Venkat directs the research efforts of several graduate students and co-workers in the Laboratory for Intelligent Process Systems. Prof. Venkatasubramanian's research contributions have been in the areas of process fault diagnosis and abnormal events management, risk identification and management in complex engineered systems, pharmaceutical engineering and informatics, molecular systems engineering, systems biology, and complex adaptive systems using knowledge-based systems, neural networks, genetic algorithms, mathematical programming and statistical approaches. His teaching interests include process design, process control, pharmaceutical engineering, systems biology, artificial intelligence, statistical physics, and applied statistics.

Prof. Venkatasubramanian has published over 165 refereed papers, and delivered over 125 invited lectures and seminars, including fourteen keynote/plenary lectures, at various international conferences and institutions all over the world. He has authored a three-volume CACHE case study on Knowledge-based Systems for Heuristic Classification Problems in Process Engineering. He has also co-authored a book on Advanced Knowledge Representation and Handbook of Diffusion and Thermal Properties of Polymers and Polymer Solutions. Venkat has been the co-editor of two books. His recent co-edited book on Computer Aided Molecular Design was published by Elsevier in 2002. Venkat has chaired or co-chaired over thirty international meetings, conferences and sessions in the areas of artificial intelligence applications in process engineering. Twenty two Doctoral and seven Masters students have graduated under Venkat's supervision. Venkat has been a consultant to several major global corporations and institutions such as Air Products, ALCOA, American Cyanamid, Arthur D. Little, Amoco, Caterpillar, Dow Agro Sciences, Eli Lilly, Exxon, GE, Honeywell, Lubrizol, United Nations (UNIDO and UNDP), Indian Oil, ICI (U.K.), Nova Chemicals, G.D. Searle (Pfizer) and others.

Prof. Venkatasubramanian's contributions have been recognized by several awards and honors. He was the 1990 recipient of the Eminent Overseas Lectureship Award from the Institution of Engineers in Australia. He was a guest co-editor of the Special Issue of Computers and Chemical Engineering on Neural Networks in 1992. In 1993, he was

awarded the United Nations Development Program Invited Lectureship at the Indian Institute of Technology, Delhi, India. Venkat is equally dedicated to teaching, and has received the Norris Shreve Award for Outstanding Teaching in Chemical Engineering in 1993, 2004 and 2006, and the Teaching for Tomorrow Award in 2004, both awarded by Purdue University. He is an academic trustee and past-President of the Computer Aids for Chemical Engineering (CACHE) Corporation, a non-profit organization for the promotion of computers in chemical engineering education. He served on the editorial board of the Process Safety Progress. He currently serves on the Editorial Board of Computers and Chemical Engineering. In 1996, Industry week magazine selected him as "one of the fifty R&D stars in the United States whose achievements are shaping the future of our industrial culture and America's technology policy". His co-authored paper on fault diagnosis was awarded the CAST Directors' Award for the Best Poster Presentation at the AIChE Annual meeting in Los Angeles, Nov 2000. Recently, Venkat and his students were awarded the Best Paper Prize for 2002-05 from the Journal of Engineering Applications of Artificial Intelligence, sponsored by the International Federation of Automatic Control (IFAC), for a paper on abnormal events detection and process risk management. He is a co-recipient of the Team Research Excellence Award from the College of Engineering, Purdue University, in 2007 for his contributions to the development of the discovery informatics framework for molecular products design. Recently, his co-authored paper on informatics won the 2006 Best Paper Prize from Computers and Chemical Engineering. In 2007, Venkat was recognized for his outstanding teaching contributions at Purdue as the only faculty member in the College of Engineering to be elected as a Fellow of the Teaching Academy.