University of Waterloo
Department of Chemical Engineering

Department of Chemical Engineering Seminar
Wednesday, July 10, 2013, 3; 30-4:30
Room: E6-2024 (Coffee and Donuts served at 3:20)

Cross Canada Tour Lecture
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Science & Engineering of Pores, Particles and Interfaces: Forays into Development of Clean and Green Processes

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We have been fascinated by phenomena occurring at the boundaries which has grown over the years with confluence of chemical and biological sciences and engineering, the formation of nanoparticles, pores and the interfaces residing within them. On one hand, network models and percolation processes in reservoir rocks, enhanced oil recovery and coal gasification, hydrogen generation to the finer aspects of multiphase reaction engineering and Green Chemistry. There is a very interesting thread among this areas which can be broadly viewed as Science & Engineering of Pores, Particles and Interfaces to develop clean and green processes, whether physical, chemical or biological or otherwise.

In recent years, my group has been working in three different areas of Green Chemistry using heterogeneous chemical catalysis, biocatalysis and phase transfer catalysis. New opportunities for the conversion of glycerol into value-added chemicals have emerged in recent years as a result of glycerol's unique structure, properties, bioavailability, and renewability. Different reaction pathways for selective catalytic conversion of bioglycerol into commodity chemicals include oxidation, hydrogenation (commonly called hydrogenolysis), dehydration, pyrolysis and gasification, steam reforming, thermal reduction into syngas, transesterification, etherification, oligomerization, polymerization, acetalization and carbonylation. The development of novel solid acids, bases, hydrogenation and oxidation catalysts for glycerol conversion will be discussed with examples. A recent area of great interest includes synthesis of enantiopure drugs, separation of racemic mixture and biocatalytic synthesis of fine chemicals. Our work encompasses different approaches to synthesize important pharmaceutical intermediates to overcome the limitations of conventional organic synthesis methods. Immobilized lipases were employed to study some pharmaceutically important reactions, under enzyme catalysis and microwave irradiation including development of kinetic models.

The liquid-liquid phase transfer catalyzed reaction can be intensified by converting it into three-liquid phases. An attractive process for the production of mandelic acid is through reaction between benzaldehyde, sodium hydroxide and chloroform in the presence of polyethylene glycol 4000 as a phase transfer catalyst. We address the modeling of a well-stirred reactor for the foregoing process in which organic droplets surrounded by a thin film of catalyst-rich phase are suspended in the aqueous phase. A population balance model is formulated L-L-L PTC reaction and solved by Monte Carlo simulation using interval of quiescence technique. Transport processes and intrinsic reaction kinetics are extracted from the experiments. This population balance model serves to assess and interpret the relative roles of various processes in L-L-L PTC reaction, such as diffusive transport, reaction and interaction between dispersed phase droplets. The model is expected to be an effective tool for reactor design and scale up.

Biographical Sketch of Professor G. D. Yadav

Professor G.D. Yadav is the **Vice Chancellor** and **R.T. Mody Distinguished Professor** of the Institute of Chemical Technology, Mumbai , and also **J.C. Bose National Fellow** (DST-GOI). He is also honoured as the Adjunct Professor at RMIT University Australia. Professor Yadav is internationally well known for his seminal and extensive contributions to **Green Chemistry and Technology, Catalytic Science and Engineering, Nanomaterials, Nanocatalysis and Biocatalysis** and for providing innovative professional leadership and yeomen services to the profession of Chemical Engineering, and Chemical and Allied Industries in India. He is an exceptional combination of leadership and academic brilliance. He has provided breakthroughs in design, synthesis and industrial applications of novel catalytic materials. He is held in high esteem by chemical and allied industry and the industrial associations. He has devised elegant selectivity engineering principles in multiphase reactions using inert nano particles, new solid superacidic catalysts, multiple liquid phases such as tri-liquid phase transfer catalysis. He has published **248 international publications** in **49 high impact factor** international journals; out of which **177** are in journals with impact factor greater than **2**. He has also authored/co-authored **3** books; and holds **53 international patents**. His work on sulfated zirconia, heteropoly acids, clays and ion-exchange resins is exceptionally well-recognized and has been cited in over **3400** papers of international repute. The **h index** of his publications now stands at **32** which is truly outstanding for an engineer-scientist. His average citations/paper and citations/year are **15.12** and **93.53**, respectively. The cumulative impact factor is **532.943**, which is again truly extraordinary for an engineer-scientist. His research is cited in **27** monographs, including the celebrated Perry's Handbook of Chemical Engineers. He has guided **61 Ph. D.** (Chemical Engineering/Technology, Biotechnology & Chemistry) and **62** Masters theses, as a single guide. These productivity statistics are remarkable.

He was the first to synthesize a solid superacid called UDCaT-5 having stronger acidity than the hitherto known sulphated zirconia (J. Catalysis, 2004), with wide spread applications. Several industrial examples have been studied with this material. His work on sulphated zirocina is a citation classic with more than **370** citations (Micro. Meso. Mater., 1999). Synergism of heteropoly acids and their modified versions and clays as nano-catalysts was brought out in his leading paper in Chemical Communications (1995), which is oft-quoted. His laboratory has reported several novel mesoporous solid superacids called UDCaTs. He has propounded the 'Selectivity Engineering Principles' in multiphase reactions very elegantly using inert nano particles, new catalysts and multiple liquid phases. He has published the pioneering theoretical and experimental proof of the celebrated phenomenon of inversion in rates and selectivity in Friedel-Crafts reactions (Tetrahdron Letters, 1993, 1995). He has introduced new concepts in phase transfer catalysis (PTC) and his work on tri-liquid PTC, the role of omega phase, and cascade engineered PTC is path-breaking (Langmuir, 2002). He also developed novel redox materials (Adv. Synth. Catal., 2008) and one of his works (OPRD, 2000) has been cited as a green method in Nobel Laureate Noyori's work on oxidations (Chem.Comm., 2003). He has also contributed to the basic work on role of microwave irradiation in catalysis including mathematical modelling (J.Mol.Cat.A,2005). Many of his papers deal with intertwining of chemistry and chemical engineering and technology. He was found to be the topmost scientist in India in the field of catalysis based on SCI database and peer reviewed papers. He is the only engineer to have figured in top 20 scientists of India as a highly productive and cited scientist with a variety of contributions to research in a survey conducted by CSIR and also DST. The hallmark of Professor Yadav's research is its focus on industrial adoption and commercialization. Some work has found extensive use in many of India's chemical manufacturing corporations. He is an active consultant to a number of industries and his research is commercialized. He is one of the highly decorated chemical engineer with several national and international honours. He has been serving on a number of important committees of central ministries and UGC, as a Chairman and as member of editorial boards of **6 international journals of repute in Catalysis**.