INTRODUCTION

The Chemical Reaction Engineering Laboratory (CREL) at Washington University in St. Louis (WUSTL) has a long tradition (over 30 years) as a premier academic institution. CREL advocates advances multiphase reaction engineering, facilitates transfer of new findings to industrial practice and educates and trains new generations of versatile reaction engineering experts with strong grasp of fundamentals.

CREL's focus on reaction engineering of multiphase systems is timeless as it addresses the basic needs of chemical engineering, a discipline involved in transformation of nonrenewable and renewable resources into fuels, chemicals, food, feed, pharmaceuticals, and new materials. It is the chemical transformations (which include biochemical, electrochemical, biological reactions) that change the structure and property of molecules generating desired products and sometimes producing by side reactions undesirable side products. The choice of reaction chemistry, catalyst, operating conditions and the selection of reactor type and contacting pattern determine the volumetric productivity, yield and selectivity of the process. An overwhelming percentage of reaction systems (over 95%) in practice are heterogeneous in nature , i.e. involve more than one phase. Quantifying reactor performance demands understanding of: 1) molecular scale events, to arrive at mechanistic description of kinetic rates, 2) microscale (single eddy, single catalyst particle scale) transport kinetic interactions, and 3) reactor scale flow patterns and phase contacting. Reactor type selection and its performance dictate the number of separation units needed in the process and their load and thus affect profoundly the overall economics of the process. The reactor is also the key to environmentally friendly processing in preventing pollution at the source.

We at the Chemical Reaction Engineering Laboratory (CREL) define reaction engineering as a powerful general methodology that quantifies the interactions between reaction kinetics (chemical, photochemical, electrochemical, biochemical, biological, etc.) and transport phenomena (momentum, mass and heat transfer) at molecular, local and global scales in various reactor types. Such quantification leads to predictive models for reactor design, scale-up/scale-down, troubleshooting and control operation.

Being an educational institution, we strive to provide a unique and stimulating environment for our students. We expect them to gain a broad knowledge of reaction engineering principles so that they can effectively use the state-of-the-art reaction engineering in a variety of diverse applications. We also require them to advance the state-of-the-art in their chosen specialty. CREL is a unique organization that strives to provide rapid transfer of academic research to industrial practice and that has developed and maintained close ties with industry. We serve our industrial sponsors in many ways: (i) by keeping them informed of the latest advances in reaction engineering, (ii) by offering access to unique experimental facilities and the best available multiphase flow models, (iii) by providing consulting services and contract work, (iv) by sending qualified students to work on company premises, (v) by offering training opportunities for industrial personnel and short courses, (vi) by doing joint research, (vii) by allowing member companies to provide input for CREL long-term research and for selection of CREL future thesis projects, and (viii) by providing our sponsors with the opportunity to leverage resources.

The current trends in industry on downsizing and increasing the efficiency and company profit margins have had many side effects. For example, even the largest companies cannot afford any more to have teams of scientists and engineers maintaining their expertise in general

areas, they are forced to specialize. Nor can the companies afford to maintain the facilities and equipment for cold flow modeling, pilot plant scale investigations or rigorous kinetic studies. Yet, the diversity of the business that they pursue and the constant pressure to scale-up new production more rapidly, or improve existing plants, require general expertise and tools for modern scale-up. CREL offers a unique opportunity to our industrial sponsors for leveraging their resources effectively. We at CREL can be a valuable partner for improved troubleshooting of existing processes and in scale-up of new ones. We also offer breadth and depth in the general methodology of reaction engineering plus some unique facilities. In this new business climate association with CREL has become an even more valuable asset to our industrial partners.

The key areas in which we offer unique services to our industrial sponsors are:

i) Quantification of flow fields, in gas-liquid, liquid-solid, gas-solid, gas-liquid-solid systems in various reactor types via our unique computer aided radioactive particle tracking (CARPT) and gamma ray computer tomography. These data are not available by other means and can be used for scale up, design and model validation. This includes further development of our novel experimental techniques (CARPT-CT) and other tools (optical probes, gas and liquid tracer techniques, heat transfer probes, mass transfer techniques, pressure fluctuation and pressure drop via differential pressure transducers, CCD camera, etc.) for measurement of flow, mixing, density profiles and transport in multiphase systems.

ii) Quantification of the reaction rate and kinetics, and evaluation and characterization of the existing, new or novel catalysts that are either in use in the existing processes and technologies or are developed for new and/or improved processes and technologies.

iii) Quantification of the impact of integrating the transport (hydrodynamics/momentum, mass and heat) and kinetics (chemistry) on the processes performance (i.e., conversion, selectivity, efficiency, safety, pollution generation, etc.).

iv) Development of advanced models for various multiphase reactor types (e.g., bubble and slurry columns, trickle beds, packed beds, stirred tanks, risers, fluidized beds, etc.) that can be coupled with client's proprietary kinetics for improved design, scale up, operation or troubleshooting of commercial and pilot plant reactors. This includes using first principles in the development of hydrodynamic and reactor models, integrating transport, hydrodynamics and kinetics and verifying such models with carefully planned experiments.

v) Validation of CFD codes by CARPT-CT and optical probe measurements in various multiphase reactor types.

vi) Development of environmentally benign process technologies (e.g. hydrocarbon oxidation, solid acid alkylations, hydrogenations, hydroformulation).

vii) Development of new concepts and reactor technology for biomass conversion to fuels and chemicals, bioprocessing and wastes treatment.

viii) Providing access to our new process concepts and ideas, facilities and expertise for potential joint projects.

ix) Inventing and investigating novel reactor types for application to environmental, biochemical and material processes.

CREL program currently encompasses: (i) quantification of flow, mixing and reaction in multiphase reactors, (ii) environmentally benign processes and beneficial catalysis, and (iii) bioreactor and bioprocessing engineering. In the area of multiphase reactors we have a unique non-invasive experimental facility that combines **Computer Automated Radioactive Particle Tracking (CARPT)** and **Computer Tomography (CT)** for measurement of instantaneous velocities, turbulence and backmixing parameters, time averaged circulation patterns and complete voidage (holdup) distribution in multiphase gas-liquid-solid, gas-liquid, liquid-solid and gas-solid systems such as bubble columns, fluidized beds, risers and stirred tanks. No other laboratory in the world has this CARPT-CT combination that provides the capabilities for studying systems with large volume fraction of the dispersed phase i.e. systems that we call opaque. Dr. M. Al-Dahhan is spearheading the effort with Oak Ridge National Laboratory, as a part of DOE funding on anaerobic digester, to advance these techniques by developing multi-particle tracking technique (MP-CARPT) and dual modality computed tomography (DMCT) for measuring simultaneously the velocity and density distribution of two/three moving phases.

Since September 1, 2003 NSF has funded our engineering research center (ERC) for excellence called "Center for Environmentally Beneficial Catalysis" (CEBC). CREL participates as a (core partner) with University of Kansas (headquarters) and University of Iowa (core partner). Through the CEBC, a new direction of research has been established in CREL which is related to development of benign processes. This involves replacing existing technologies involving environmentally hazardous chemicals and solvents with new chemistries after solvents are replaced using supercritical CO_2 or a mixture of solvent and supercritical CO_2 called "expanded bed or solvent" (Drs. M.P. Dudukovic, M.H. Al-Dahhan and P.A. Ramachandran). Dr. Jay Turner supervises the education planning and effort set for CEBC. In addition, research area related to the biofuel processing, namely ethanol production from corn, has been initiated in collaboration with National Corn to Ethanol Center (NCEC) of the Southern Illinois University (SIUE) – Edwardsville (Drs. M.P. Dudukovic, M.H. Al-Dahhan, C. Charpenter). The activities of the newly established research focus area within CREL, have been in progress as a part of CREL called "Bioreactors and Bioprocesses Engineering Laboratory (BBEL)" headed and formed by Dr. M. Al-Dahhan. In CREL, Dr. M. Al-Dahhan continues to spearhead the effort on high pressure bubble/slurry bubble column and also examining the use of multiphase systems as bioreactors such as trickle-beds, packed bubble columns (non-structured and structured packing), stirred tanks, liquid-solid and gas-solid circulating systems, with special attention dedicated to photobioreactors, biodigesters, and waste water treatment processes. Dr. P.A. Ramachandran continues to broaden both the CREL computational base and know-how in multiphase reactors. All research projects in CREL stress advances in fundamentals but applications are always sought in areas of specific interest to our sponsors.

Work in CREL has been initiated to package the results of a multiyear modeling effort in CREL on various multiphase reactors into user friendly software/programs that can be easily used by students, engineers, scientist, and operators in industry.

CREL has continued its international interactions with a number of national and world renowned university laboratories dealing with various aspects of multiphase systems such as those at the Ohio State University, Rensselaer Polytechnique University, University of Delft, and Twente University in Holland, University of Norway at Trondheim, University of Stuttgart, University of Hannover and Dresden University in Germany, ENSIC at Nancy in France, Waterloo University, Ecole Polytechnic and Laval University in Canada, National

Technical University of Athens in Greece, Almeria University in Spain and the National Chemical Laboratory in Pune, India. We intend to expand such interactions in the forthcoming years.

The continuity of our research in reaction engineering has been made possible by the **Department of Energy (DOE), NSF, USDA and our industrial sponsors**. In 2004/2005 they are: **Air Products, BP, Chevron Texaco, Conoco Phillips, DuPont, Eastman, Eni Technologie, Exxon-Mobil, IFP, Innovene, Johnson Matthey, Praxair, Sasol, Shell, Statoil, Syntroleum, Total, and UOP**. To them goes our gratitude for having the foresight to support fundamental and applied research in the areas that are vital to their businesses.

As is customary, we report here only on the **NON-PROPRIETARY WORK** executed under government or general CREL consortium funding. Results of specific industrial contract research work are reported only to the individual sponsors until released for dissemination to CREL general sponsors and ultimately for publication.

We would like to alert our sponsors that an effective way of advancing their research objectives is to enter into mini consortia or super membership agreements with CREL. **Both the mini consortium and super membership are described in the next section.** We have such an arrangement with ConocoPhillips, EniTechnologies, Sasol and Statoil for the high pressure slurry bubble column work. In the past we had such arrangement with Bayer. We are seeking interested parties for a mini-consortium on multiphase stirred tank reactors. Recently, we established such relationship with Innovene (a new company that split from BP). We are currently seeking members to form **a mini-consortium for advancing the knowledge and understanding of the gas-solid riser and fluidization**. Resources in this project were leveraged by CREL participation in the Multiphase Fluid Dynamic Consortium (MFDRC) which was funded by Department of Energy Office of Industrial Technology (DOE-OIT) and industry. We are, as well, looking for partners for our **reactive-catalytic distillation initiative**. CREL would like to extend our current rate based models and develop an experimental facility for rapid testing and scale-up of the combined catalytic reactor-distillation concept. We have also initiated a new project on the development of minireactors for oxidation and alkylation processes as one of NSF-CEBC projects **for which we are seeking partners from industry**. Finally, we are looking for companies interested in supporting research in **liquid phase oxidation of organics**. **In this area we have received three patents and equipment from Praxair and one patent from Shell of which we have notified our sponsors**. The donated patents and experimental facility are related to Liquid Oxidation Reactor (LOR), a reactor technology that can benefit the production of aromatic acids, especially terephthalic acid. The patents improve LOR aromatic acids production by switching from air as the oxidant in the process to oxygen or to oxygen enriched air. The equipment and process technology covered by the patents allow safe and efficient use of oxygen in the reactions. In addition, we are currently seeking members to either form a mini-consortium to advance the understanding, know-how and design of LOR processes using LOR and CREL advanced measurement techniques, or to negotiate a bilateral arrangement. **(Recently, a new project on liquid oxidation of organics to produce TPA (Teriphthalic acid) using Praxair and Shell patents and the impact of supercritical CO_2 on the process efficiency and product quality has been initiated as part of NSF-CEBC oxidation projects for which we are also seeking industrial partners through CEBC membership).**

While this Introduction mainly describes past events and touches only lightly on the future, we would like to use this opportunity **to alert our sponsors that we have enhanced our**

advanced control capabilities via most modern virtual and actual laboratory, hardware and software. **Greg McMillan**, retired senior fellow at Solutia, spearheaded our efforts based on the HYSYS platform (part of ASPEN) and with Emerson's Delta V system. This facility is available for training and education of personnel at member companies. We also have **Terry Tolliver** and **Bob Heider** involved with our control initiative.

Finally, executive CREL board has been formed during 2004 CREL Annual Meeting to work on establishing a strategic and business plans for CREL present and future directions and interactions with industry and governmental funded agencies. The recommendations of this board will be presented and discussed with CREL sponsors for their comments and feedback.