Welcome to the
30-th Meeting of the
Chemical Reaction Engineering Laboratory (CREL) and Industry
October 6, 2005

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http://crelonweb.che.wustl.edu
The domain of chemical engineering consists of chemical and physical transformation (as well as biological) of starting materials to products.

The key to economically and environmentally friendly process is in choosing the right chemical transformations and right reactor type and being able to scale them up.
Use of Multiphase Reactor Technology

Syn & Natural Gas Conversion
- MeOH, DME, MTBE, Paraffins, Olefins, Higher alcohols, ...

Petroleum Refining
- HDS, HDN, HDM, Dewaxing Fuels, Aromatics, Olefins, ...

Value of Shipments: $US 637,877 Million

Polymer Manufacture
- Polycarbonates, PPO, Polyolefins, Specialty plastics

Bulk Chemicals
- Aldehydes, Alcohols, Amines, Acids, Esters, LAB’s, Inorg Acids, ...

Environmental Remediation
- De-NOx, De-SOx, HCFC’s, DPA, “Green” Processes...

Fine Chemicals & Pharmaceuticals
- Ag Chem, Dyes, Fragrances, Flavors, Nutraceuticals, ...

Biomass Conversion
- Syngas, Methanol, Ethanol, Oils, High Value Added Products

Chemical Reaction Engineering (CRE) Methodology: Multi-scale Quantification of Kinetic-Transport Interactions

Reactor performance affects number and size of separation units and overall economics of the process.
ADVANCES IN MULTIPHASE REACTORS REQUIRE:

a) capturing the physics of flow by experimental means
b) doing CFD models and validating the results experimentally
c) completing physically based engineering models for flow and mixing.

REACTOR SCALE MODELS FOR CONTACTING OF TWO MOVING PHASES

Ideal Reactor Concepts:

A) Plug Flow (PFR)

B) Stirred Tank (CSTR)

C) Axial Dispersion Model

D) Need More Accurate Flow & Mixing Description Via
   Phenomenological models based on:
   1) CFD Models (Euler-Euler Formulation)
   2) Experimental Validation: Holdup Distribution and Velocity Field

Dudukovic, AI CHE Symposium Ser., 321, 30-50 (1999)
Dudukovic, Larachi, Mills, Catalysis Reviews (2002), 44(1), 123-246
Validation of CFD for Multiphase Systems and Improved Model Development for Scale-Up, Design and Troubleshooting

Computer Automated Radioactive Particle Tracking (CARPT) and Gamma Ray Computed Tomography (CT) yield the flow map of phase distribution and velocity in various systems:

- Bubble columns (slurry)
- Liquid-solid risers
- Moving beds
- Ebulated beds

Advances in CARPT-CT technology

Process Applications

<table>
<thead>
<tr>
<th>Computer Automated Radioactive Particle Tracking (CARPT)</th>
<th>Computed Tomography (CT)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="High Pressure Bubble Column" /></td>
<td><img src="image2.png" alt="Normal Pressure Bubble Column" /></td>
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</tbody>
</table>
CREL Objectives

• Education and training of students
• Advancement of reaction engineering methodology
• Transfer of state-of-the-art reaction engineering to industrial practice

CREL Funding

• General industrial CREL participation fees
• Federal grants
• Industrial mini-consortium
• Federal contracts
• Specific contract work
• Specific training
CREL Deliverables to Sponsors

- Annual report
- Annual meeting
- Copies of theses and reports prior to publication
- Training of personnel on CREL premises
- Networking with high quality institutions
- Access to unique experimental facilities
- Contract research work and reports
- Troubleshooting and consulting
- Opportunity to leverage resources
Need Enhanced CREL – Industry Cooperative Efforts

- Development of generic experimental and modeling tools for specific multiphase reactors or systems.
- Development of models and database for specific reactor types or for specific technology (mini-consortia, GOALI and other grants, sales and service contracts)
- Development of new technology (research contracts with / without government involvement)
- Closer ties on specific research projects (industrial co-advisors of student theses)

Energy and biomass conversion are some obvious candidates for CREL involvement.
Initial CREL Executive Advisory Board Charged with Mapping out Future CREL Organization and Interaction with Industry

- Hugh Stitt (Johnson Matthey)
- Bernie Toseland (Air Products)
- Tiby Leib (DuPont)
- Paul Sechrist (UOP)
- Stan Proctor (Consultant / Ex-Monsanto)

Please provide them with your suggestions during this meeting for more effective CREL –industry interactions and for better ways for supporting CREL research.

Also suggest methods for selecting Board members.
Acknowledgement of Significant Past CREL Contributions

N. Devanathan - CARPT - Bubble Columns
Y. Yang - CARPT - Bubble Columns
B.S. Zou - CARPT - Bubble Columns
S. Kumar - CT-CARPT - Bubble Columns
S. Limtrakul - CT-CARPT - Bubble Columns
B. Sannaes - CARPT - Bubble Columns
S. Degaleesan - CARPT - Bubble Columns
J. Chen - CARPT-CT - Bubble Columns, Packed Beds
S. Roy - CARPT-CT - Bubble Columns
A. Kemoun - CARPT-CT - Bubble Columns
A. Rammohan - CARPT-CT - Slurry Bubble Columns
N. Rados - CARPT-CT - Slurry Bubble Columns
B.C. Ong - CARPT-CT - Bubble Columns

CARPT-CT

CFD, Reactor Models & Experiments

K. Myers - Bubble Columns
R. Holub - Trickle Beds
B.S. Zhou - Tap Reactor Model
S. Pirooz - Plasma Reactors
V. Kalthod - Bioreactors
H. Erk - Phase Change Regenerators
A. Basic - Rotating Packed Bed
M. Al-Dahhan - Trickle Beds
J. Turner - Fly Ash and Pollution Abatement
S. Karur - Computational CRE
M. Kulkarni - Reverse Flow in REGAS
Q. Wang - Bubble Columns
Z. Xu - Photocatalytic Distillation
K. Balakrishnan - Computational CRE
M. Khadilkar - CFD, Models, Trickle Beds
Y. Jiang - CFD, Models, Trickle Beds
J-H. Lee - Models, Catalytic Distillation
Y. Wu - Models (Trickle Beds, Bubble Column)
Y. Pan - CFD (Bubble Columns)
P. Gupta - Models (Bubble Columns)
P. Chen - Bubble Columns
Center for Environmentally Beneficial Catalysis

Designing environmentally responsible molecules, products, and processes – from the molecular scale to the plant scale.

**Lead Institution:** University of Kansas (KU)

**Core Partners:** University of Iowa (UI); Washington University in St. Louis (WUStL); Prairie View A&M University (PVAMU)

**Director:** Bala Subramaniam (KU); **Deputy Director:** Daryle Busch (KU)

**Associate Directors:** John Rosazza (UI); Milorad Dudukovic (WUStL); Irvin Osborne-Lee (PVAMU)
Environmentally Beneficial Catalytic Engineered Systems

TG1: Catalyst Design and Preparation

TG2: Media and Catalyst Supports

TG3: Experimental Design and Advanced Measurements

TG4: Multi-scale Process Model
- Quantum effects
- Molecular dynamics
- Rate theories
- Solvent thermodynamics and kinetic effect
- Micromixing
- Multi-component transport
- Turbulence
- Mixing
- Computational fluid dynamics
- Reactor simulation
- Plant simulation
- Control
- Optimization

CEBC – U. of Kansas, U. of Iowa, CREL-WU
Near-Term (5 Yr) Goals

Develop transformational catalytic technologies using CEBC’s strategic research concept for the following classes of reaction systems (termed as *testbeds*)

– Selective oxidations
– Oxidative biocatalysis
– Hydroformylations of olefins
– Solid acid catalyzed alkylations & acylations
# 2005 CREL ANNUAL MEETING

## AGENDA

**Thursday, October 6, 2005**

**Place:** Washington University – Hilltop Campus (Knight Executive Center)

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<tr>
<th>Time</th>
<th>Event</th>
<th>Presenter/Company</th>
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<tr>
<td>8:30 – 8:45 a.m.</td>
<td>Welcome Remarks</td>
<td>M.P. Dudukovic</td>
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<td>8:45 – 9:15 a.m.</td>
<td>Microreaction Engineering: Is Small Really Better?</td>
<td>Jan Lerou - Velocys</td>
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<td>9:15 – 9:45 a.m.</td>
<td>Applications of Computational Fluid Dynamics in the Process Industries</td>
<td>Peter Spicka - Fluent</td>
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<td>9:45 – 10:15 a.m.</td>
<td>Corn Biorefineries – Overview of Current Status and Future Directions</td>
<td>Charles Abbas - ADM</td>
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<td>10:15 – 10:30 a.m.</td>
<td>Coffee Break</td>
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<td>10:30 – 11:00 a.m.</td>
<td>A Status Report on Multiphase CFD for Gas-Particles Systems</td>
<td>Tom O’Brien – NETL/DOE</td>
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<td>11:00 – 12:30 p.m.</td>
<td>Introduction of Posters and New Technologies</td>
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<td>12:30 – 1:30 p.m.</td>
<td>Lunch</td>
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<td>1:30 – 5:00 p.m.</td>
<td>Viewing of Posters, Discussion of New Technologies and Laboratory Visits</td>
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<td>3:00 – 3:45 p.m.</td>
<td>CREL Facility Tour</td>
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<td>5:00 – 6:00 p.m.</td>
<td>Discussion of CREL’s Future Directions and Industrial Needs - with all participants</td>
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<td>6:00 – 6:45 p.m.</td>
<td>Reception</td>
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<td>6:45 – 8:15 p.m.</td>
<td>Dinner</td>
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<tr>
<td>8:15 – 9:15 p.m.</td>
<td>Making Friends with Chemical Reactors</td>
<td>O. Levenspiel</td>
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<tr>
<td>9:15 – 10:00 p.m.</td>
<td>Ad hoc Discussion</td>
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**Note:**

*Meeting of CREL Executive Advisory Board: Friday, Oct. 6th at 8:30am – Urbauer Hall 208

*Short Course: Friday and Saturday, Oct. 7th-8th, 2005 – Urbauer Hall 218
  “Introduction to Multiphase Reactors”, Dr. Patrick Mills (DuPont) and CREL Faculty*