Washington
WASHINGTON · UNIVERSITY · IN · ST · LOUIS
School of Engineering & Applied Science

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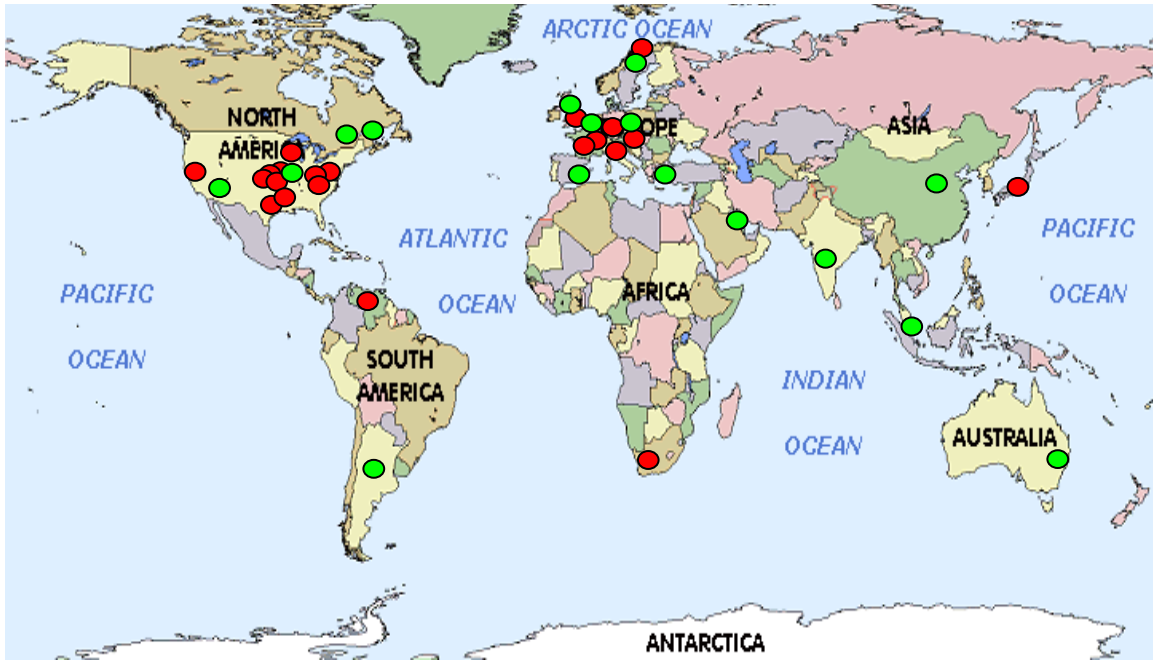
Welcome to the

30-th Meeting of the Chemical Reaction Engineering Laboratory (CREL) and Industry

October 6, 2005



● Sponsors
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INDUSTRIAL SPONSORS 2004/05

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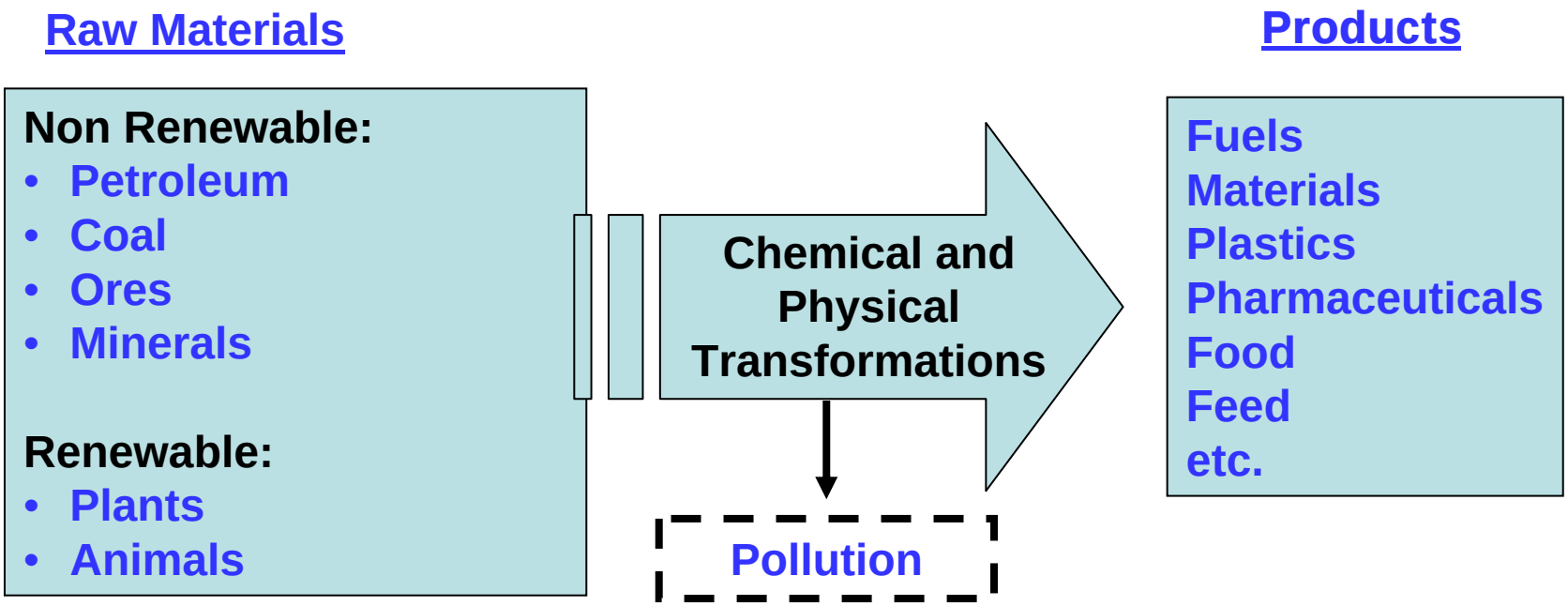
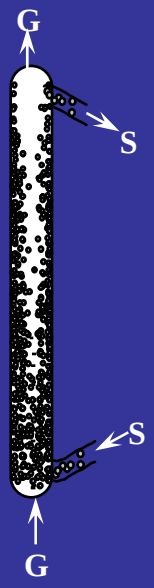
PRAXAIR
SASOL
SHELL
STATOIL
TOTAL
UOP

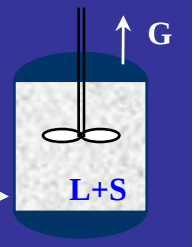
The domain of chemical engineering consists of chemical and physical transformation (as well as biological) of starting materials to products



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, ...

Bulk Chemicals

Aldehydes, Alcohols, Amines, Acids, Esters, LAB's, Inorg Acids, ...

Value of Shipments: $US 637,877 Million

Polymer Manufacture

Polycarbonates, PPO, Polyolefins, Specialty plastics

Fine Chemicals & Pharmaceuticals

Ag Chem, Dyes, Fragrances, Flavors, Nutraceuticals,...

Biomass Conversion

Syngas, Methanol, Ethanol, Oils, High Value Added Products

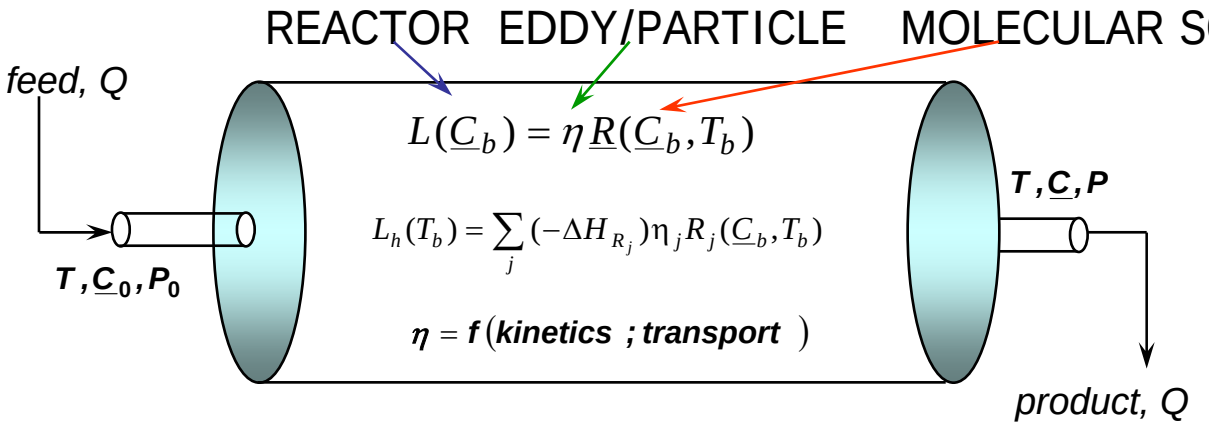
Environmental Remediation

De-NOx, De-SOx, HCFC's, DPA, "Green" Processes ..

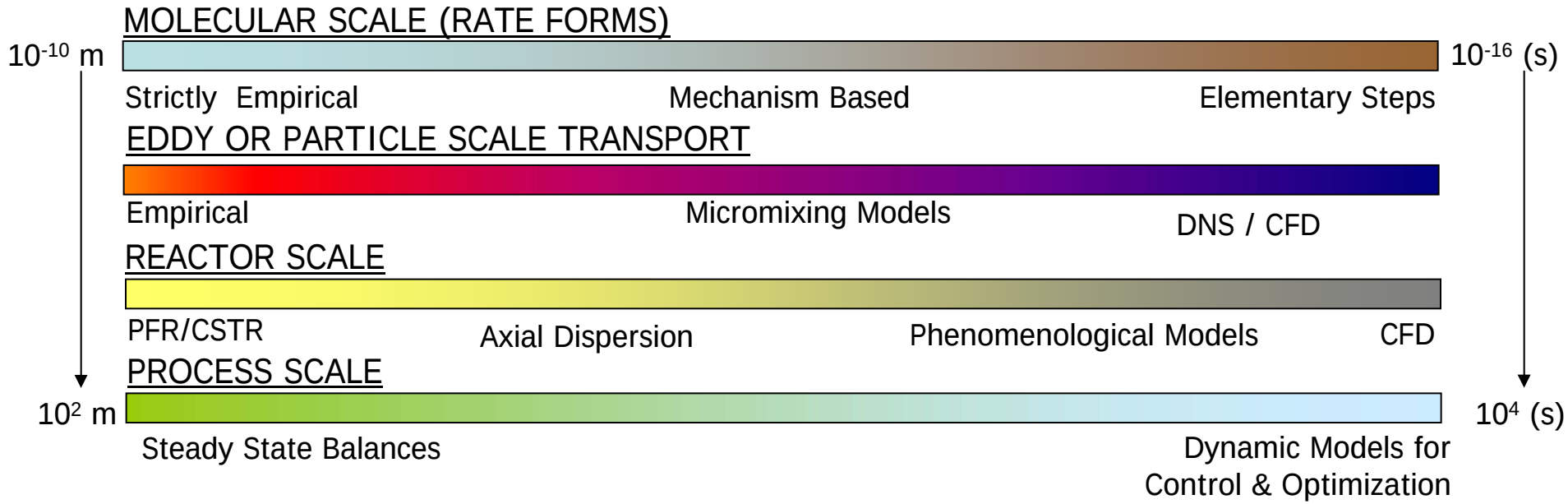
Dudukovic, Mills, Larachi, Catalysis Reviews, 44(1), 123-246 (2002)

CHEMICAL REACTION ENGINEERING (CRE) METHODOLOGY:

Multi-scale Quantification of Kinetic-Transport Interactions



REACTOR PERFORMANCE = f (input & operating variables ; rates ; mixing pattern)



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..

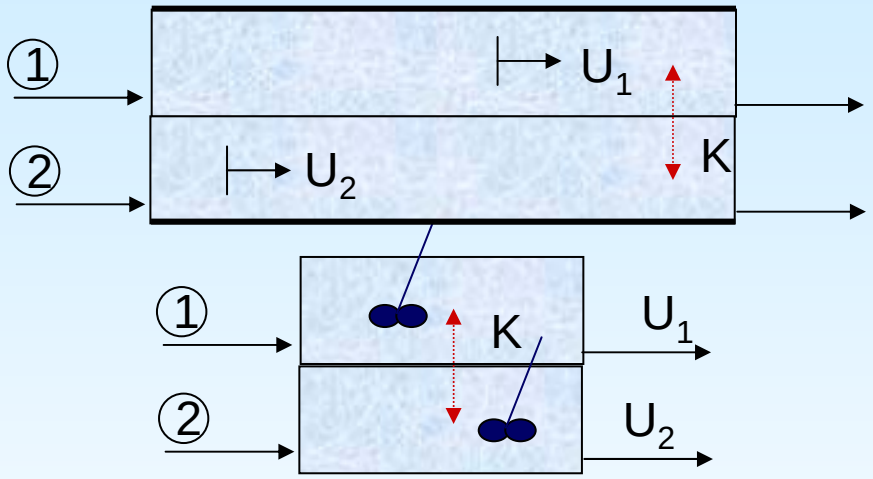
REACTOR SCALE MODELS FOR CONTACTING OF TWO MOVING PHASES

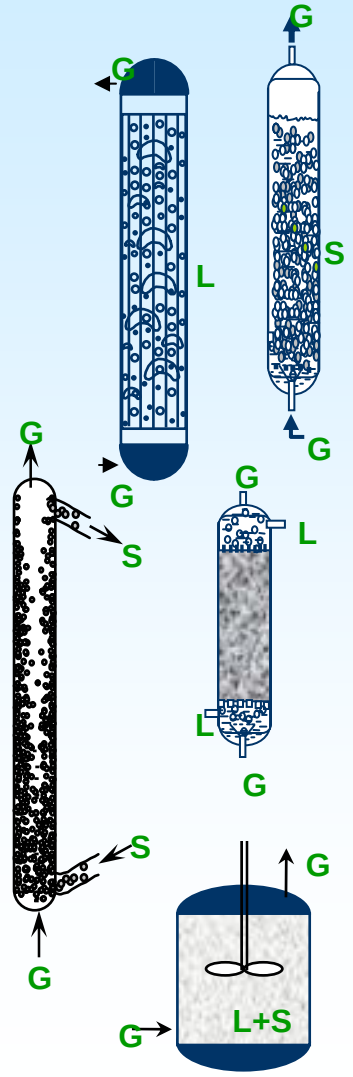
Ideal Reactor Concepts:

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, AICHE 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

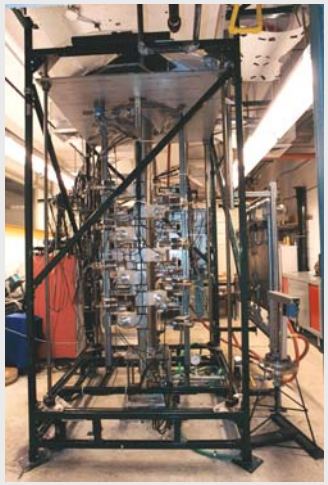
- **Bubble columns (slurry)**
- **Liquid-solid risers**
- **Moving beds**
- **Ebulated beds**

- **Gas-solid riser**
- **Stirred tanks**
- **Trickle beds**
- **Monoliths with two phase flow**
- **Fluidized beds**

Advances in CARPT-CT technology

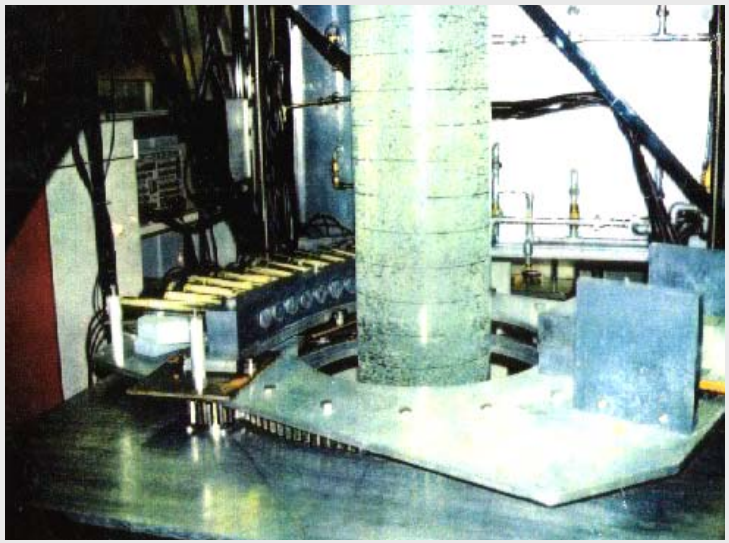
Process Applications

Computer Automated Radioactive Particle Tracking (CARPT)



High Pressure Bubble Column

Computed Tomography (CT)



Normal Pressure Bubble Column

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 memebrs.

Acknowledgement of Significant Past CREL Contributions

CARPT-CT

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	-	Ebulated Beds
B. Sannaes	-	CARPT	-	Slurry Bubble Columns
S. Degaleesan	-	CARPT	-	Bubble Columns
J. Chen	-	CARPT-CT	-	Bubble Columns, Packed Beds
S. Roy	-	CARPT-CT	-	Liquid-Solid Riser
A. Kemoun	-	CARPT-CT	-	Riser, Stirred Tank
A. Rammohan	-	CARPT-CT	-	Stirred Tank
N. Rados	-	CARPT-CT	-	Slurry Bubble Columns
B.C. Ong	-	CARPT-CT	-	Bubble Columns

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

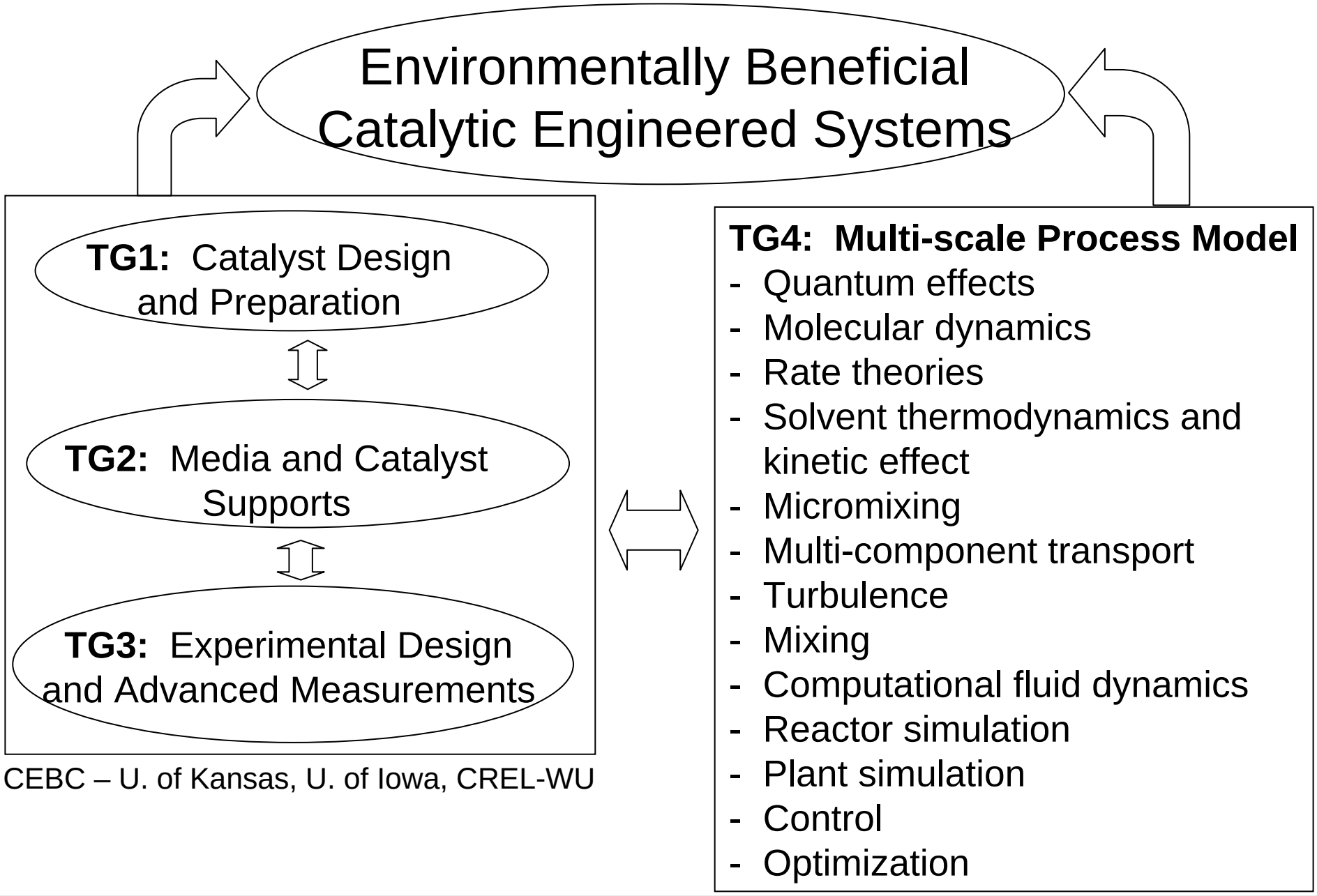
Designing environmentally responsible molecules, products, and processes – from the molecular scale to the plant scale.

***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)**



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)

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

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