INTRODUCTION TO CREL

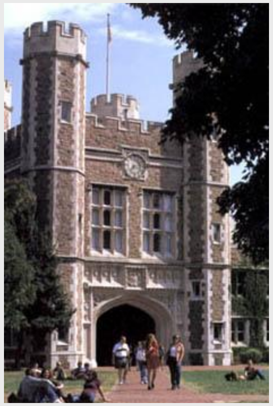
M.P. Dudukovic

Chemical Reaction Engineering Laboratory (CREL)

http://crelonweb.wustl.edu

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

Washington University Facts



- The University is ranked 11th in 2005 USN&WR for full-time undergraduate education
- $480 million was received in total research support, including $414 million in federal obligations. *
- The National Science Foundation ranked Washington University 6th among major private universities and 13th among all universities. *
- The University ranks 5th among all educational institutions receiving research support from the National Institutes of Health (NIH), and the School of Medicine ranks 3rd among all medical schools. *
- 2,911 total instructional faculty *
- 10,462 total full-time students *
- 3,357 total degrees awarded * The School of Engineering represents 25% of the Bachelor’s degrees

*** Fiscal 2003**

Washington

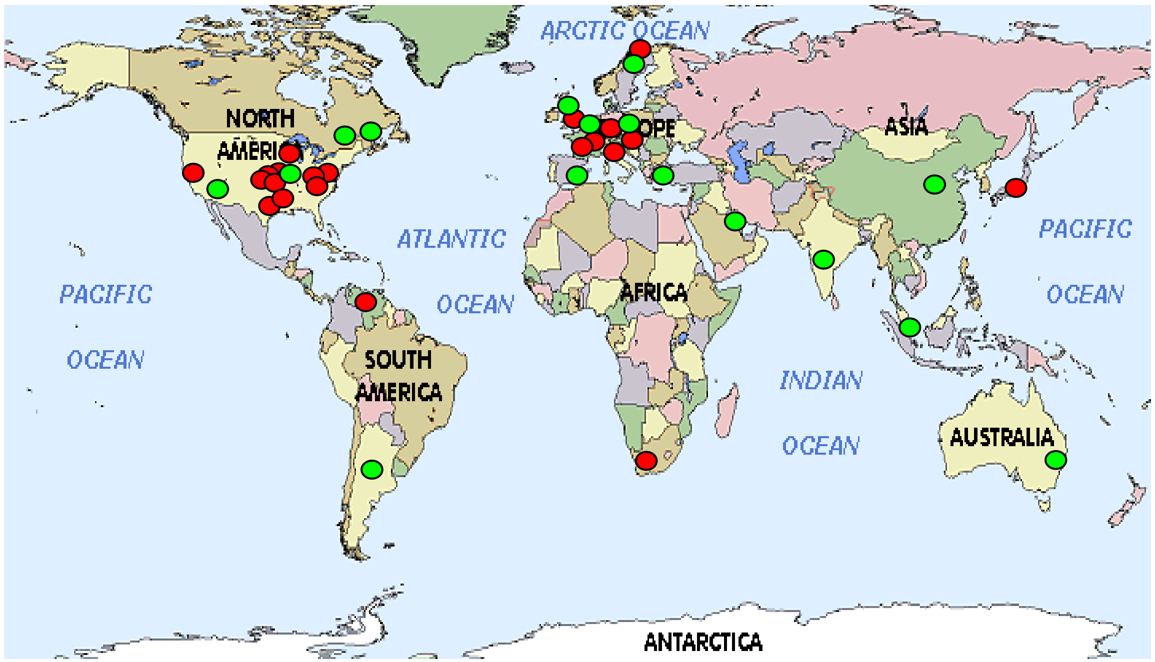
WASHINGTON · UNIVERSITY · IN · ST · LOUIS

School of Engineering & Applied Science

Welcome to the

29th Meeting of the Chemical Reaction Engineering Laboratory (CREL) and Industry

October 28, 2004



● Sponsors
● Collaborators

INDUSTRIAL SPONSORS 2003/04

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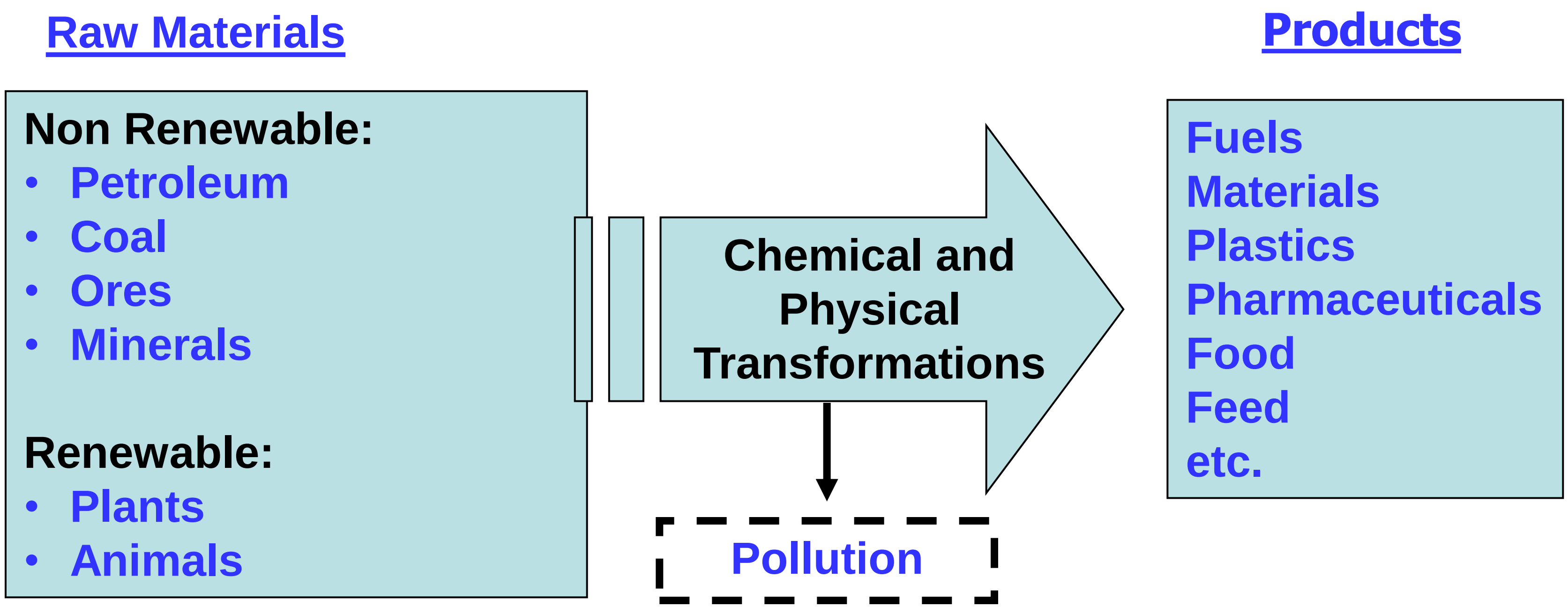
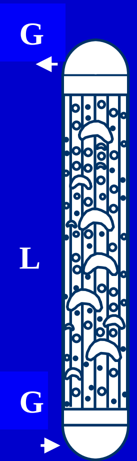
The domain of chemical engineering consists of chemical and physical transformation of starting materials to products



Key to economically and environmentally friendly process is in choosing the right chemical transformations and being able to scale them up.

Use of Multiphase Reactor Technology

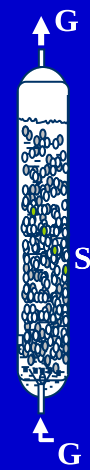


Syn & Natural Gas Conversion

MeOH, DME, MTBE, Paraffins, Olefins, Higher alcohols, ….

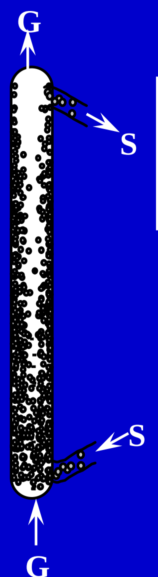
Petroleum Refining

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

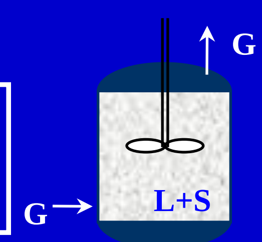
Ag Chem, Dyes, Fragrances, Flavors, Nutraceuticals,...

Biomass Conversion

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

Environmental Remediation

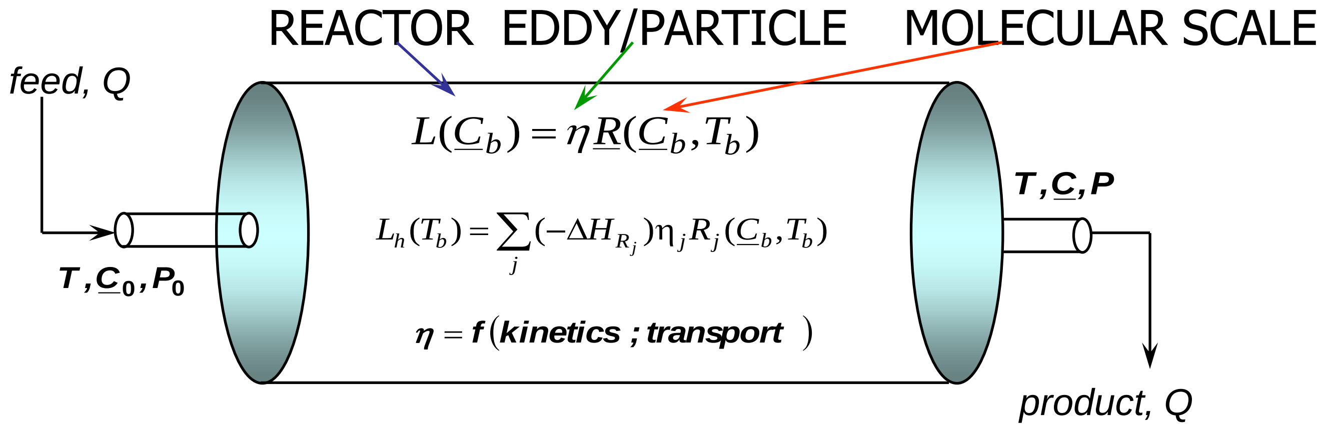
De-NOx, De-SOx, HCFC's, DPA, "Green" Processes ..



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)

10^{-10} m → 10^{2} m ; 10^{-16} (s) → 10^{4} (s)

MOLECULAR SCALE (RATE FORMS)

Strictly Empirical — Mechanism Based — Elementary Steps

EDDY OR PARTICLE SCALE TRANSPORT

Empirical — Micromixing Models — DNS / CFD

REACTOR SCALE

PFR/CSTR — Axial Dispersion — Phenomenological Models — CFD

PROCESS SCALE

Steady State Balances — Dynamic Models for Control & Optimization

Reactor performance affects number and size of separation units and overall economics of the process

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 Activities

- Exploration of novel process concepts and of new technology
- Development of improved multiphase reactor models and validation of CFD models for multiphase reactors for
  - Scale-up and design
  - Troubleshooting
- Development of toolboxes and turn-key models and training of personnel

Sources of Novel Process Concepts

1. Conceptual ideas (Main source: Dr. Walter Knox)
   - Biomass to syngas
   - Syngas to vinyl acetate, methyl vinyl chloride, ethanol
   - Propylene oxide from propane, oxygen and hydrogen
   - Isobutane to p-xylene
   - Methane to methanol
   - Methane to ethanol
   - Biomass and/or coal to hydrogen
   - Methane to acetic acid
   - Etc.

2. John Gleaves' novel catalyst development for selective oxidations (butane to maleic, propylene to acrolein, acrolein to acrylic), oxidative hydrogenation (propane to propylene), epoxidation (propylene to propylene epoxide), etc.

3. CEBC (Center for Environmentally Beneficial Catalysis – NSF ERC)
   - Solid acid alkylation and acetylation
   - Partial oxidation (cyclohexane to cyclohexanone and cyclohexanol or direct to Acetic Acid)

Novel Multiphase Reactor Technology

1. Microreactor Technology (Mikroglas - Invenios)
   - Safe manufacture of explosive materials
   - Determination of key process variables in oxidations and other gas-liquid reactions

2. LOR (Liquid Oxidation Reactor Technology)
   - Use of increased oxygen concentration (or pure oxygen) in teraphthalic acid manufacture
   - Extension of LOR to other oxidations

3. Biazzi Hydrogenation Technology

4. Ultra Short Contact Time Reactors and Reactor - Regenerators

Validation of CFD for Multiphase Systems and Improved Model Development for Scale-Up, Design and Troubleshooting

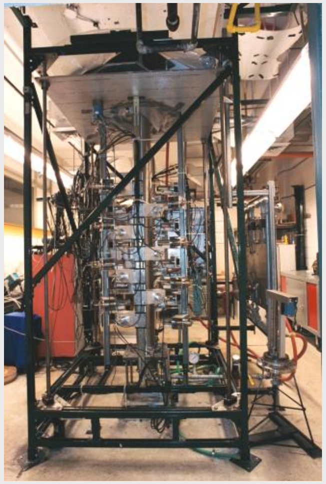
Computer Automated Radioactive Particle Tracking (CARPT) and Gamma Ray Computed Tomography (CT) yield the flow map of phase distribution and velocity in various systems

- Bubble columns (slurry)
- Liquid-solid risers
- Moving beds
- Ebulated beds
- Gas-solid riser
- Stirred tanks
- Trickle beds
- Monoliths with two phase flow
- Etc

Advances in CARPT-CT technology

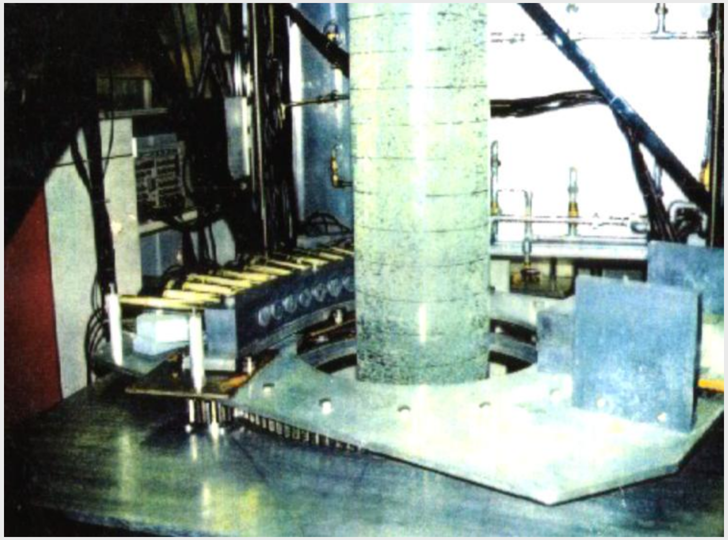
Process Applications

Computer Automated Radioactive Particle Tracking (CARPT)



High Pressure Bubble Column

Computed Tomography (CT)

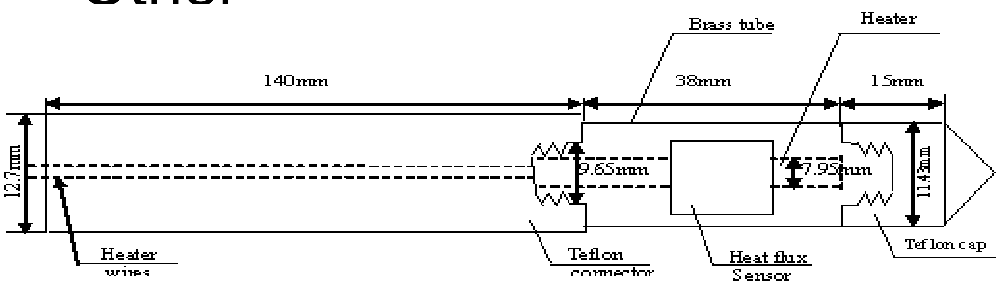


Normal Pressure Bubble Column

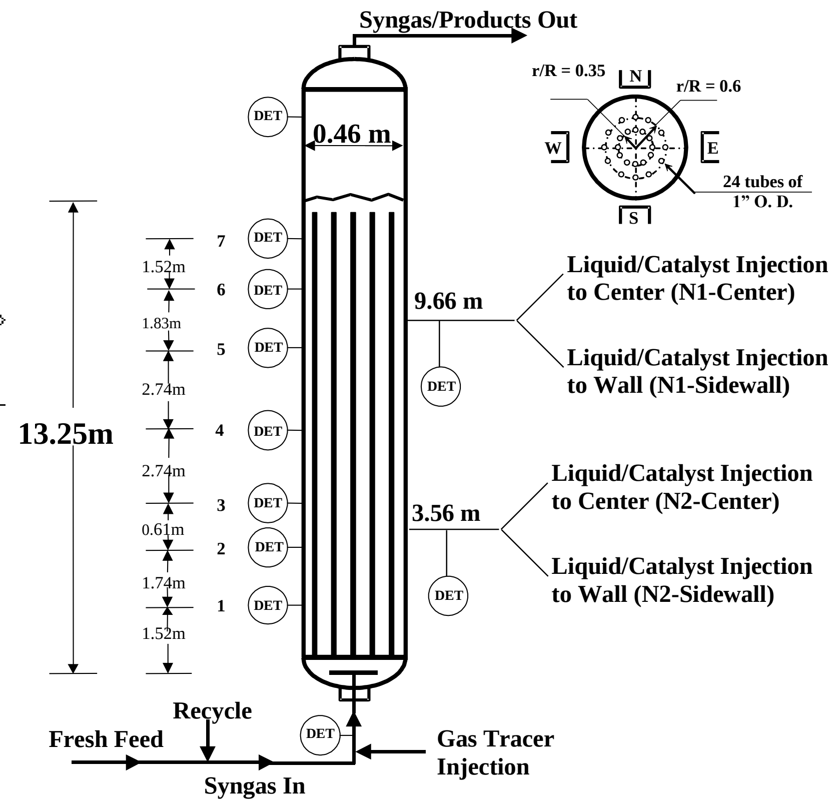
Scale-Up Models

Point probes:

- Optical probes (bubble dynamics)
- Mass transfer
- Real transfer
- Other



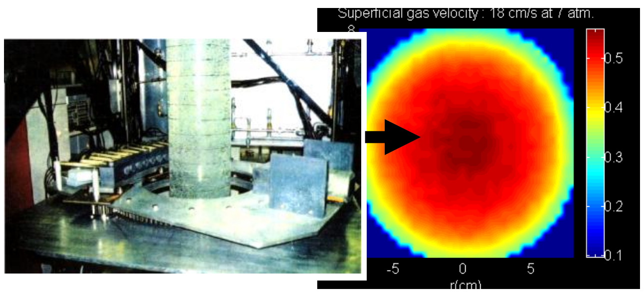
- Troubleshooting: Gamma ray densitometry, tomography, tracer methods



For sound scale-up and design strategy one needs validated CFD codes. CARPT-CT are used to develop an appropriate reactor flow and mixing model. CFD generated data are used to assess model parameters. Reactor flow and mixing model is coupled with the kinetic information.

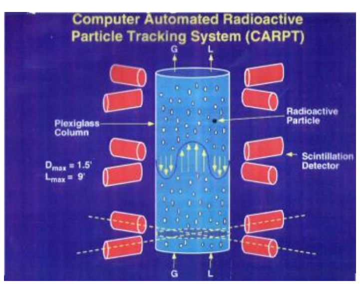
Degaleesan et al., Chem. Eng. Sci., 51, 1967(1996); I&EC Research, 36,4670 (1997); Gupta et al., Chem. Eng. Sci., 56, 1117 (2001); Peng and Dudukovic, Chem. Eng. Sci. (submitted 2004).

Bubble Column Example

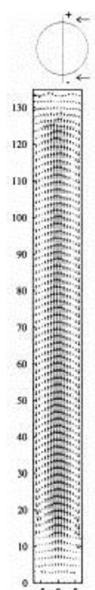


CT **CT SCAN**

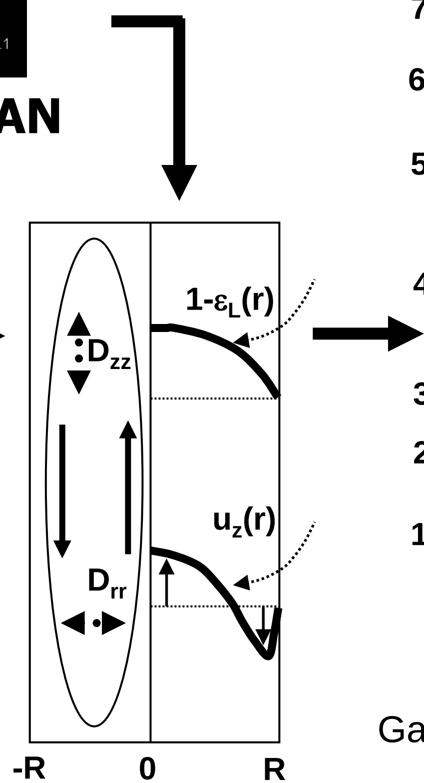
CFD + CARPT + CT

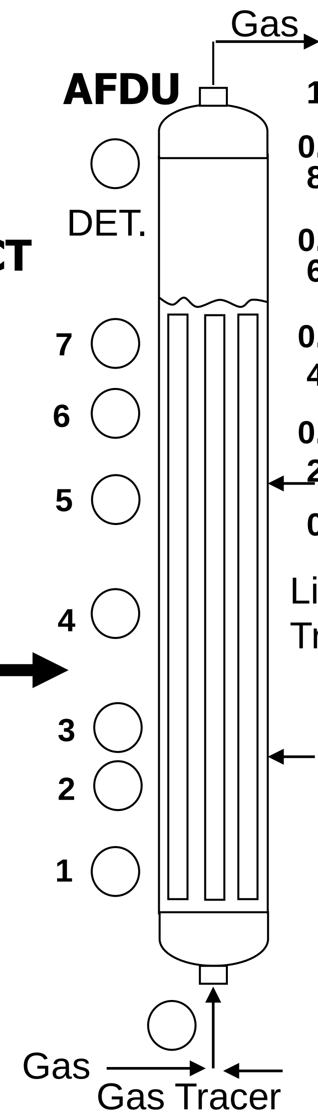


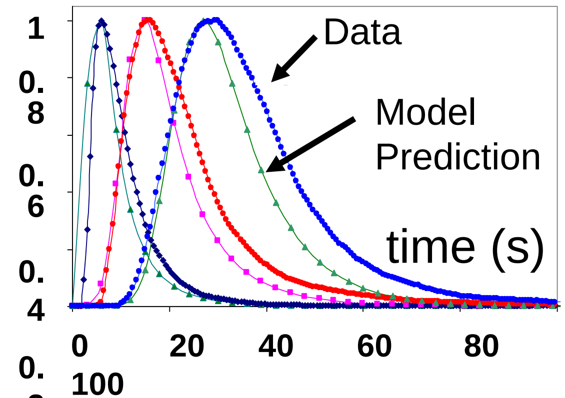
CARPT

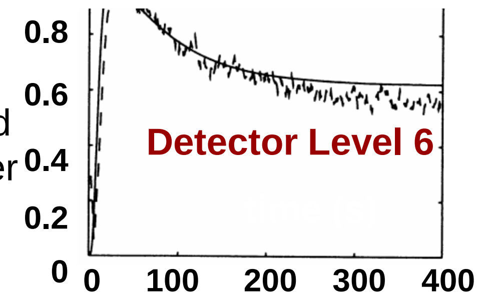


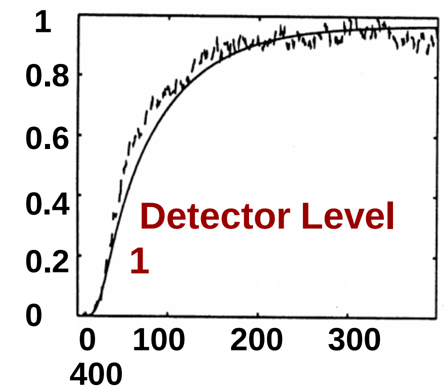
FLOW PATTERN









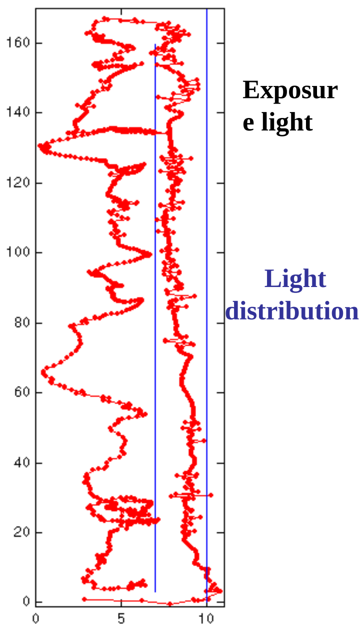


Process Development, Turn-Key Models, Tool Boxes

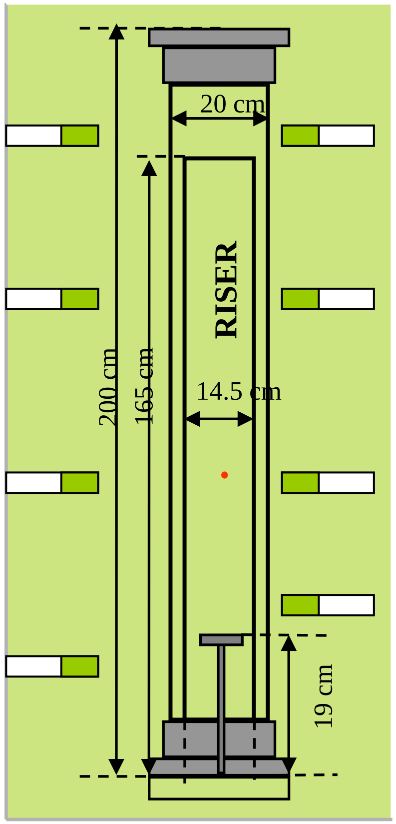
- Corn – to – ethanol for NCRC at SIUE (USDA funded)
- Anaerobic digester design and operation (DOE funded)
- Airlift reactor for photo induced algal growth (CREL funded)
- Other proprietary contracts!

Application: Photobioreactor Algal Growth

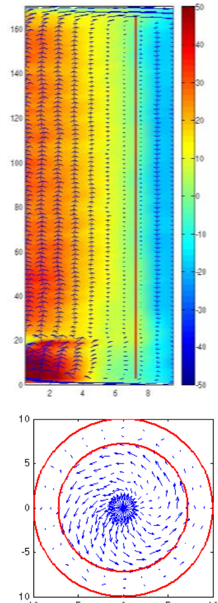
Airlift Bioreactor



Cells' Movement

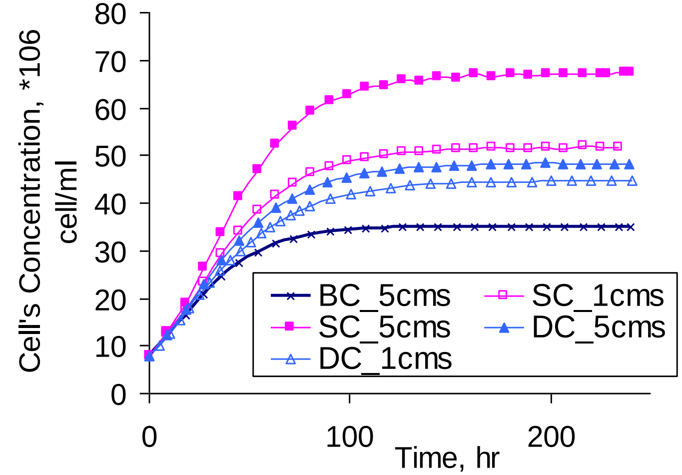


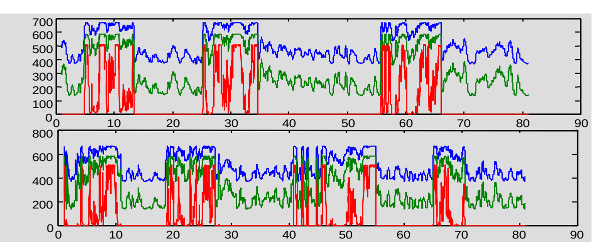
Flow Visualization



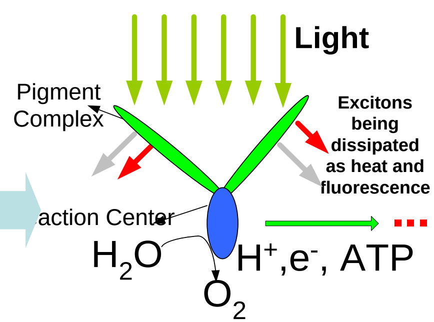
Luo and Al Dahhan(2003)

(BC: Bubble Column; SC: Split airlift column; DC: Draft tube airlift column)

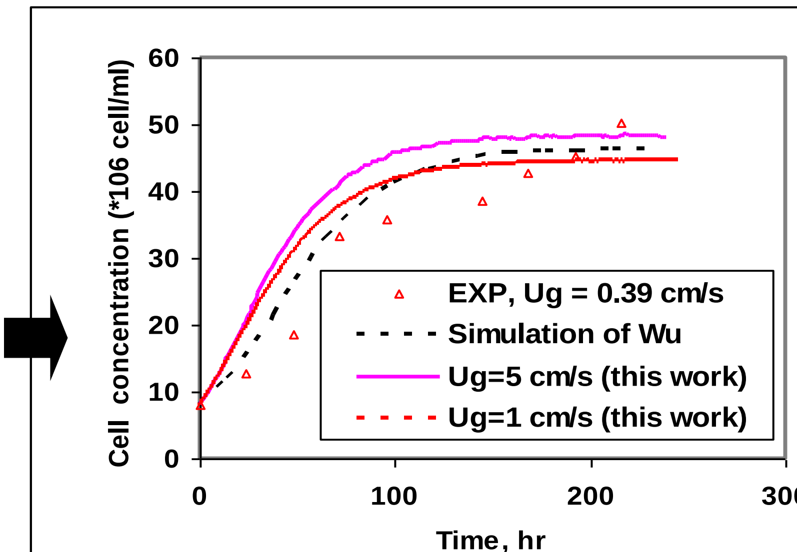




Time Series of Light intensity experienced by the Cells in the reactor



Physiologically Based Photosynthesis rate model



Dynamic Simulation

CREL Deliverables to Sponsors

- Annual report
- Annual meeting
- Copies of theses and reports prior to publication
- Training of personnel on CREL premises
- Joint proposals to federal funding agencies
- 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 multiphase 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)

To maximize value that CREL brings to sponsors and provide for continuity of research we need to:

- Identify person(s) responsible for authorizing CREL participation fee in each company
- Explore raising the fee to expand company participation in multi-institutional or multinational effort (e.g. CEBC, NCL, etc.)
- Appoint an industrial executive advisory board to offer advice on use of CREL general funds and spearhead special initiatives
- Identify at each company people who can connect CREL to company planned government funded initiatives (via DOE-ATP, OIT, etc.)
- Give CREL and its partners a chance to participate in new process development for the company.

CREL Advisory Board

Selected representatives or participating companies are current CREL advisors.

Company representatives advising D.Sc. Students are appointed in addition as adjunct faculty.

Need Executive Advisory Board

- To define its role, functions, election of members
- To focus on enhancing CREL value to industry
- To enhance opportunities for CREL funding

Initial Executive Advisory Board

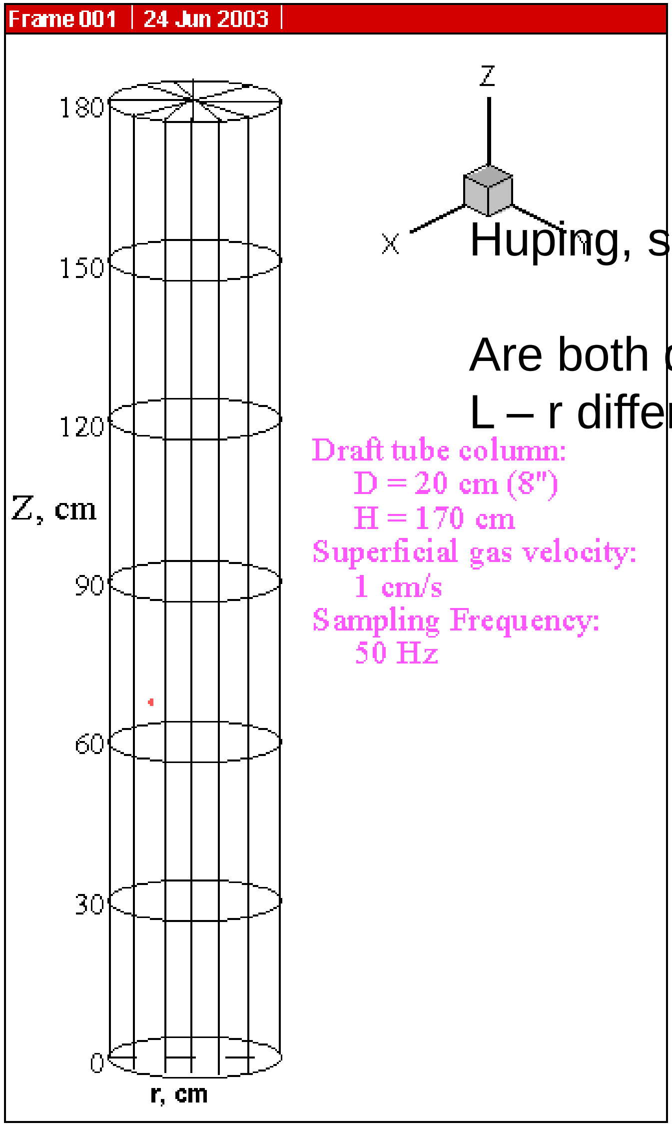
- Hugh Stitt (Johnson Matthey)
- Bernie Toseland (Air Products)
- Tiby Leib (DuPont)
- Stan Proctor (Consultant / Ex-Monsanto)

Organizational meeting with all industrial representatives

Thursday, October 28, 2004

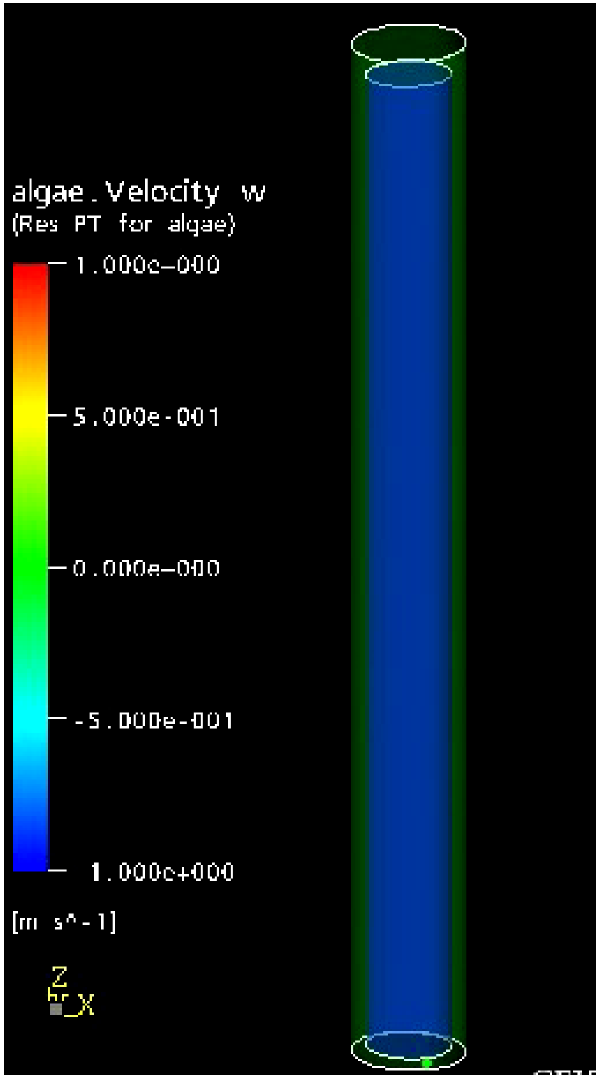
4:00 p.m.

Radioactive Particle Tracking –
A good way to get velocity information in opaque systems



Huping, specify conditions

Are both draft tube columns
L – r differnece?



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

ACKNOWLEDGMENTS

Department of Energy:	**DE-FC22 95 95051** **DE-FG22 95 P 95512**
CREL Industrial Sponsors:	**ABB Lummus, Air Products, Bayer, Chevron, Conoco, Dow Chemicals, DuPont, Elf Atofina, Exxon, EniTechnologie, IFP, Intevep, MEMC, Mitsubishi, Mobil, Monsanto, Sasol, Shell, Solutia, Statoil, Synetix, Union Carbide, UOP**
CREL Colleagues and Graduate Students:	**M.H. Al-Dahhan, J. Chen, S. Degaleesan, N. Devanathan, P. Gupta, A. Kemoun, B.C. Ong, Y. Pan, N. Rados, S. Roy, A. Rammohan, Y. Jiang, M. Khadilkar**
Special Thanks to:	**B.A. Toseland, Air Products and Chemicals** **M. Chang, ExxonMobil** **J. Sanyal, FLUENT, USA** **B. Kashiwa, CFDLib, Los Alamos** **V. Ranade, NCL, Pune, India**

2003 CREL ANNUAL MEETING

AGENDA

Thursday, October 28, 2004

Place: Washington University – Hilltop Campus (Knight Executive Center – Room 220)

8:30 – 9:00 a.m.	**Welcome and Introduction - M.P. Dudukovic**
9:00 – 9:40 a.m.	**The Importance of Fundamentals in the Future Directions for the Chemical Industries - Kurt Vanden Bussche (UOP)**
9:40 – 10:20 a.m.	**Utilizing Fundamentals in Design, Scale-up and Troubleshooting - Hugh Stitt (Johnson-Matthey)**
10:20 – 10:40 a.m.	**Coffee Break**
10:40 – 11:20 a.m.	**Reactor, Process and Product Engineering via Flow Modeling - Vivek Ranade (NCL)**
***11:20 – 12:40 p.m.**	**Introduction of Posters and New Technologies**
12:40 – 2:00 p.m.	**Lunch**
****2:00 – 4:30 p.m.**	**Viewing of Posters, Discussion of New Technologies and Laboratory Visits**
4:30 – 5:30 p.m.	**Future Directions and Needs (Industrial Participants Only)**
5:30 – 6:00 p.m.	**Meeting of Industrial Advisory Board with CREL**
6:00 – 6:45 p.m.	**Reception**
6:45 – 8:15 p.m.	**Dinner**
8:15 – 9:15 p.m.	**The Story of Chemical Reaction Engineering - O. Levenspiel (Oregon State University)**
9:15 – 10:00 p.m.	**Ad hoc Discussions**

*** New Technologies**

Mikroglas Microreactor system (www.invenios.com)

Biazzi Hydrogenation Reactor – Direct scale up from lab to production size (www.biazzi.com)

****CREL Facility Tours**

1. 1:45 – 2:30 p.m.