Multiscale Reaction Engineering for Clean Energy and Environment

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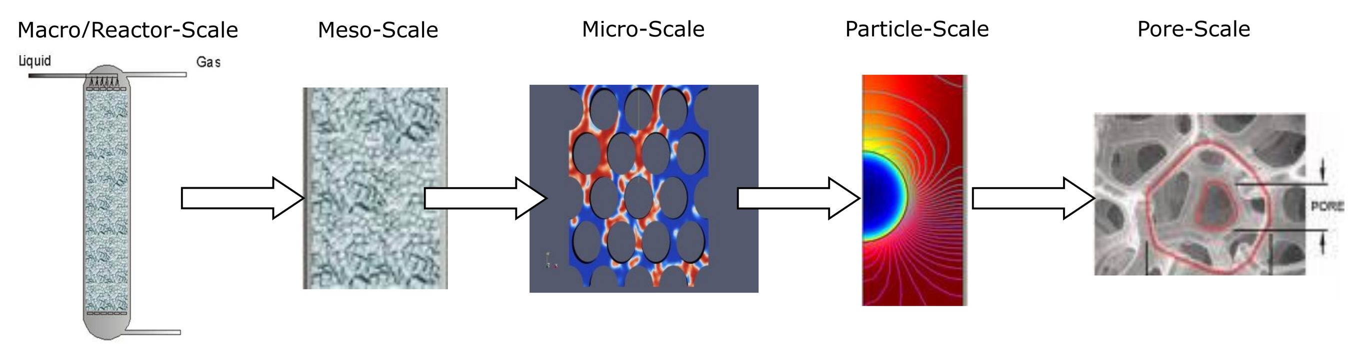
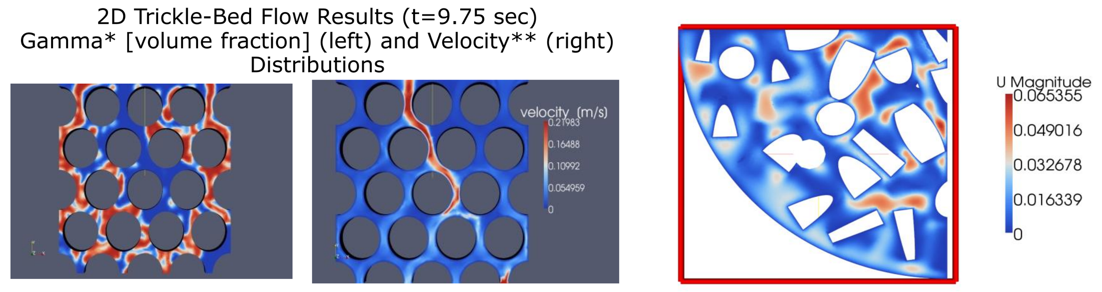
Multiscale Modeling of Packed Beds

Dan Combest



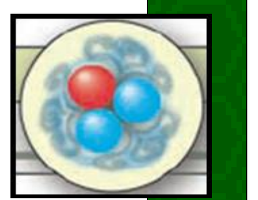
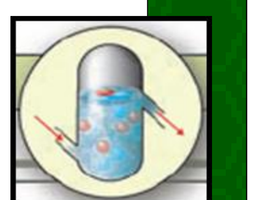
Current modeling resolves heat, mass, and momentum transport near catalyst surfaces and interstitial spaces over a domain of 10-100 catalyst particles in a packed bed. Models can be used for any process chemistry and are the building blocks for larger scale models. This level of resolution increasingly elucidates the interactions of phenomena across multiple length scales.

2D Trickle-Bed Flow Results (t=9.75 sec)
Gamma* [volume fraction] (left) and Velocity** (right) Distributions



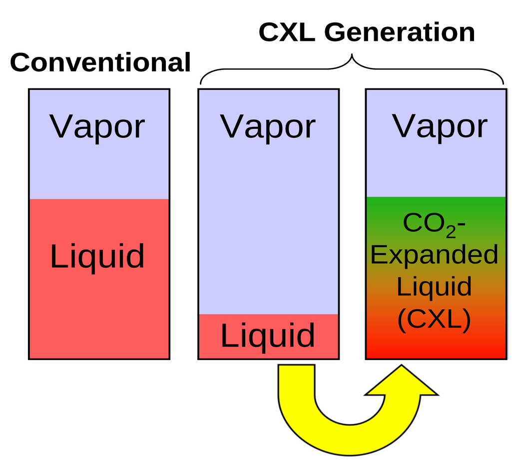
*In gamma results, red = liquid and blue = gas
**higher velocity in red, lower in blue
Horizontal cross-section Z-Velocity Profile

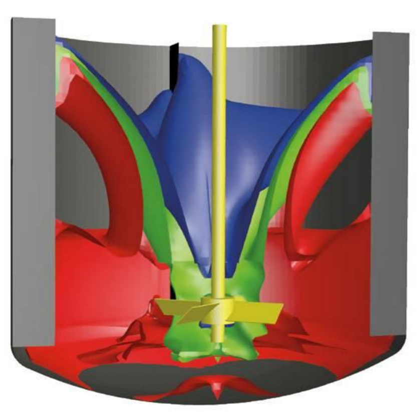
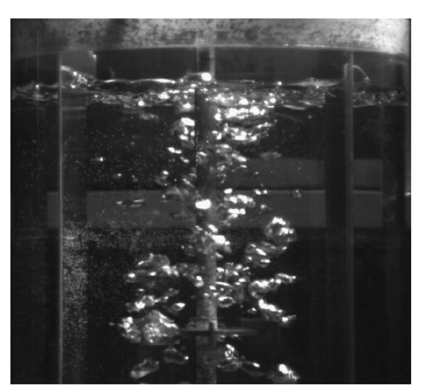
Reference: CREL Annual Report 2009-2010 Pages 23 - 26

Green Reactor Engineering by Characterization of Multiphase Flows

Dr. Sean Mueller

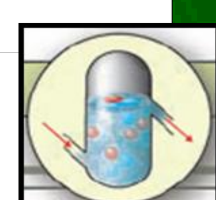


New optical probe tools quantitatively characterize fluid state and hydrodynamics in opaque, multiphase chemical reactors. These novel tools can be used in high pressure and high temperature environments commonly encountered in industry where conventional measurement techniques fail; and, they can be used as on-line process control tools.

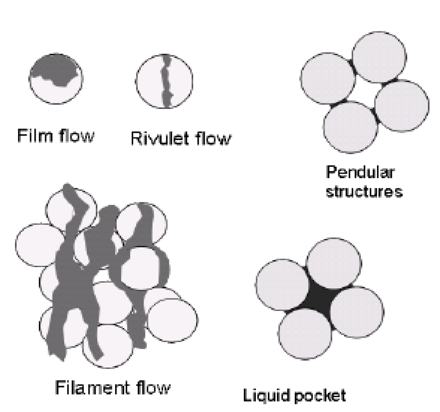
These tools characterize and evaluate emerging green processes such as hydrodgen producing bioreactors and carbon dioxide expanded liquid (CXL) reactors. For example, CXLs can replace significant amounts of harsh solvents used in industry and improve efficiency at the same time.

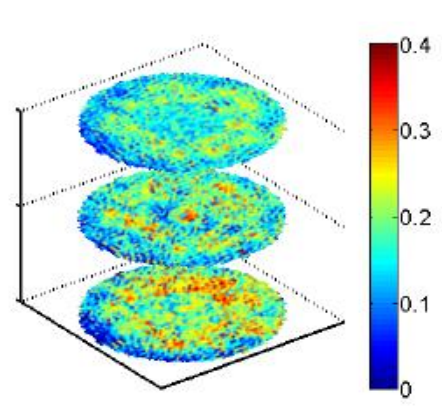
Reference: CREL Annual Report 2009-2010 Pages 46-50




Multiscale Hydrodynamics of Trickle Bed Reactors

Dr. Zeljko Kuzeljevic

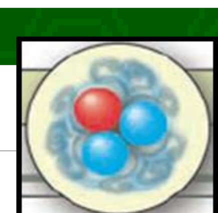
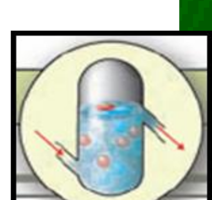




Trickle Bed Reactors (TBRs) are used in the production of fuels, waste water treatment, desulfurization, and liquid fuel synthesis from non-conventional sources.

Research focuses on the computational and experimental tools to assist us in design and scale-up of TBRs using advanced measuring techniques (e.g., computed tomography) and the Eulerian CFD simulation approach for establishing a closed form of coupling of particle scale equations (external and intraparticle mass transfer and kinetic resistances).

Reference: CREL Annual Report 2009-2010 Pages 27 - 30

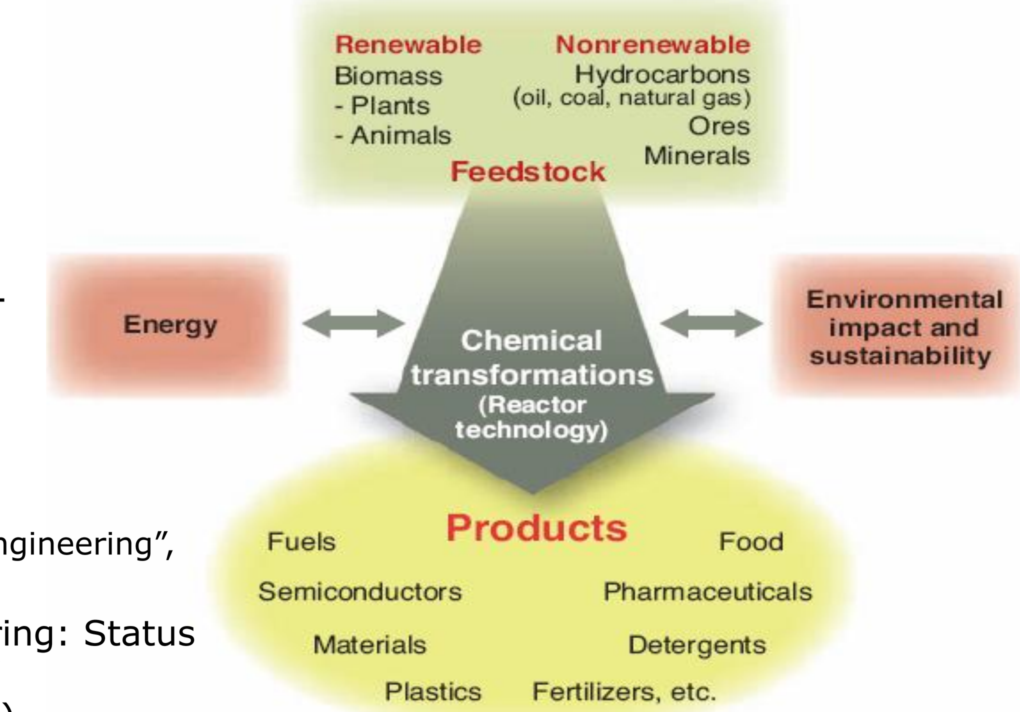

Advancing the scientific basis of multiscale kinetic transport interactions is the key to the development of green technologies

Examples of current research projects in CREL and their relation to multiscale reaction engineering are provided in this poster. For an even greater perspective you are most welcome to join the Multiscale Reaction Engineering Review today from 6-8 pm, Session V in Brauer Hall on Tuesday, and refer to our website and the following articles:

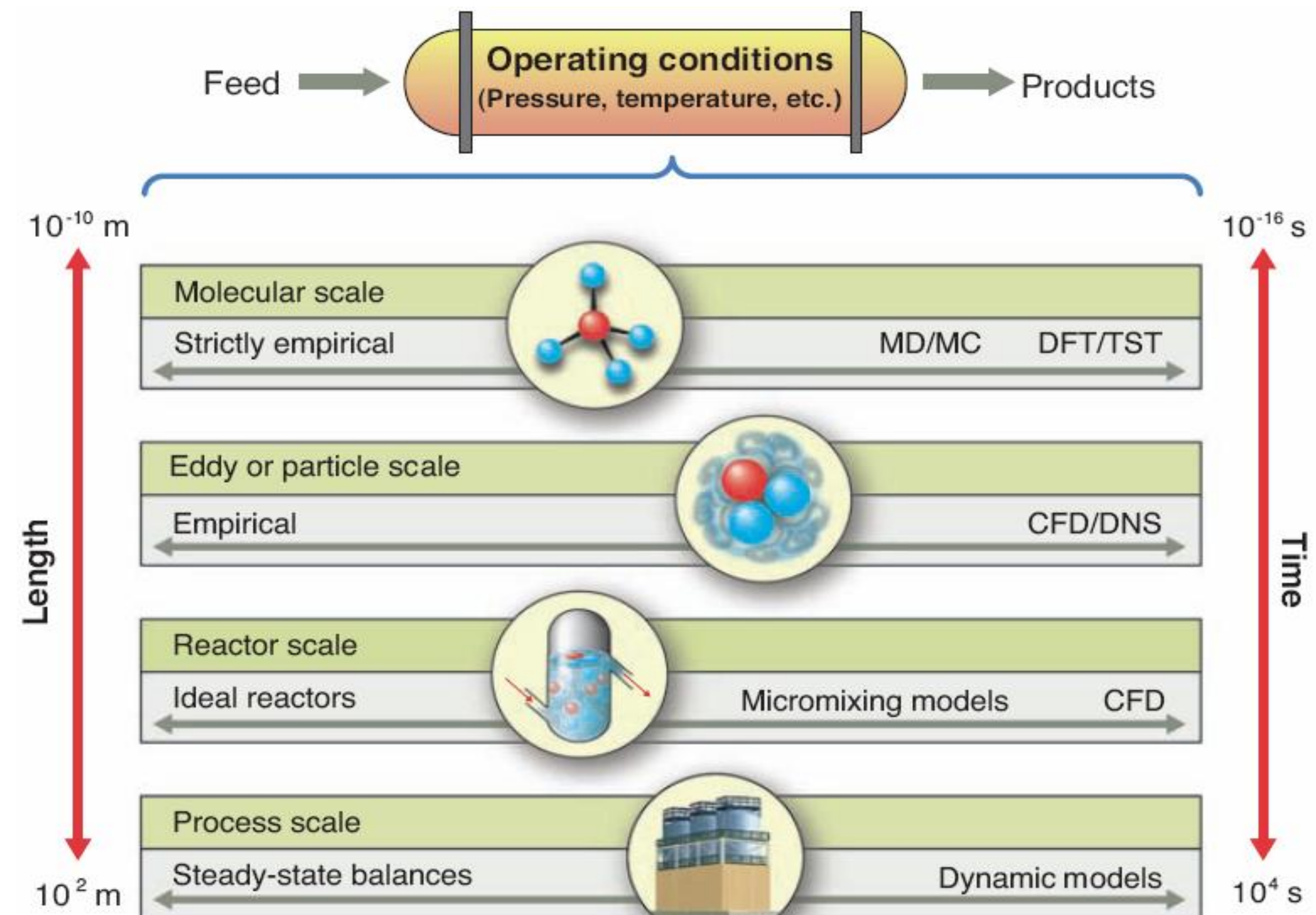
http://crelonweb.eec.wustl.edu

M. Dudukovic, "Frontiers in Reactor Engineering", *Science*, **325**, 698 (2009).

M. Dudukovic, "Reaction Engineering: Status and Future Challenges", *Chemical Engineering Science*, **65**, 3 (2009).

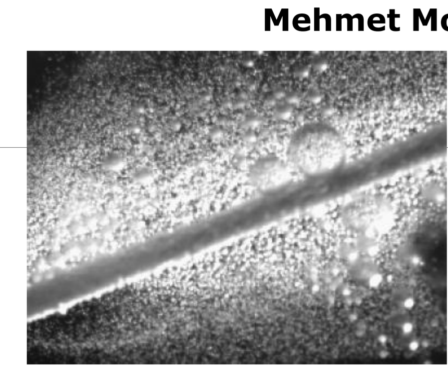


Reactor performance prediction requires quantitative modeling of various phenomena on various length/time scales. As we increase the level of scientific understanding at each scale of multiscale reaction engineering, we move farther to the right on the bars (shown below).



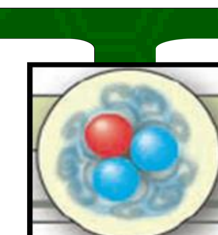
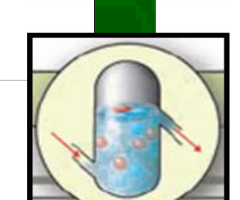
Liquid and Gas Flow in Electrochemical Systems

Mehmet Morali



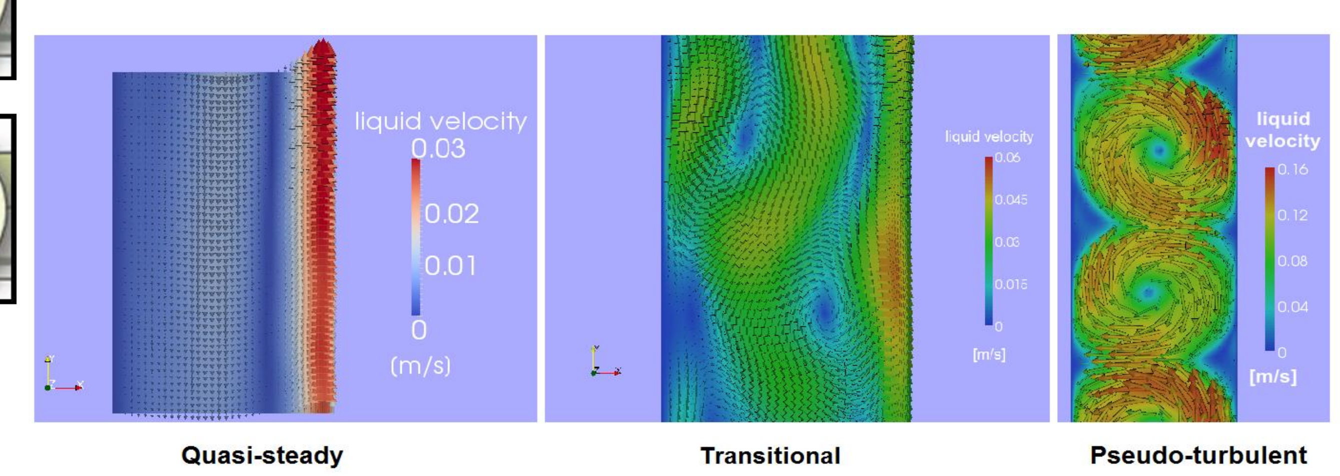

Electrochemical systems provide environmentally friendly alternatives to the production of various chemicals. To improve the efficiency of these systems, fundamental understanding of relevant multiphase phenomena is necessary. Towards this improvement, we are implementing experimental and modeling tools with emphasis on bubble flow field interaction, bubble generation on the surface and bubble coalescence in the system.

Reference: CREL Annual Report 2009-2010 Pages 54 - 56

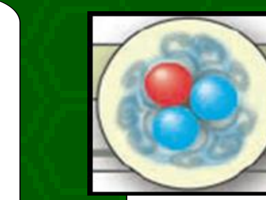
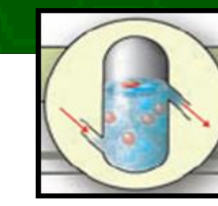
Modeling of Electrochemical Channels

Dr. Alessio Alexiadis



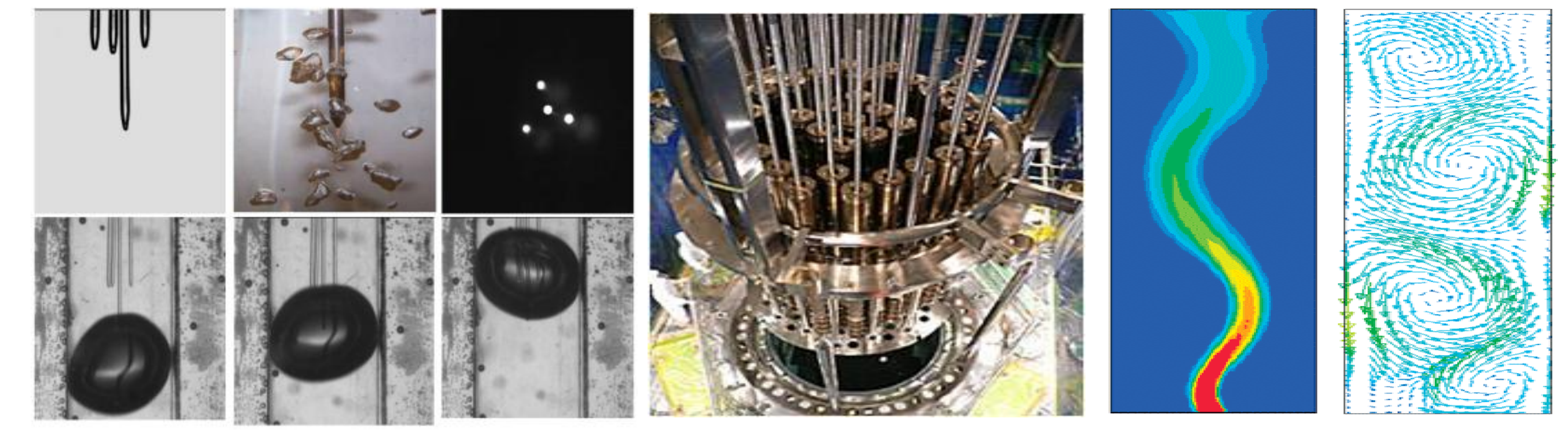
The fluid motion in an electrochemical channel depends on the bubbles generated at the electrode. Depending on the diameter (d) and the current density (i), we have various flow regimes: quasi-steady (i=1000 Am-2, d=0.1 mm), transitional (i=400 Am-2, d=0.01 mm) and pseudo-turbulent (i=1000 Am-2, d=0.01 mm). The efficiency of the system is strictly connected with the fluid-pattern of the system.

Reference: CREL Annual Report 2009-2010 Pages 51 - 53


Mixing and Mass Transfer in Bubble Columns with Internals

Mohamed Hamed



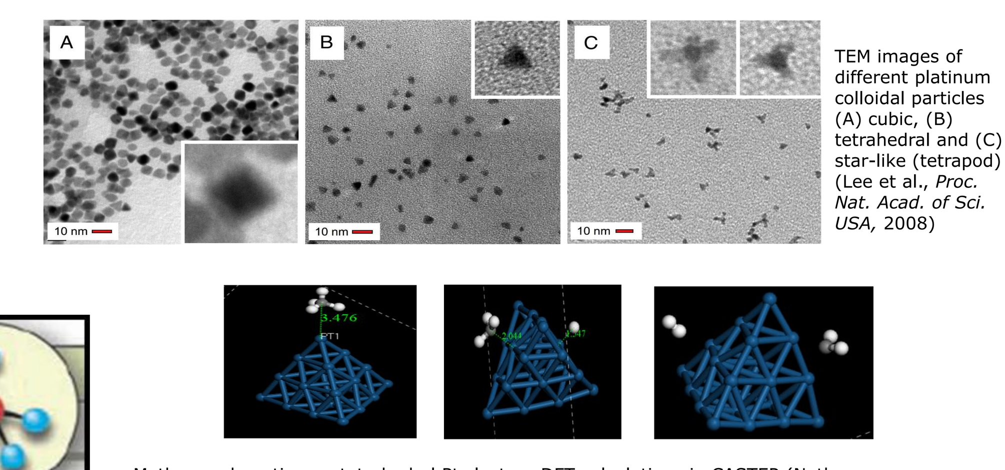
Bubble columns find applications in gas-to-liquid, biomass-to-liquid and coal-to-liquid reactors since they offer high conversion and high volumetric productivity when operated in the heterogeneous or churn turbulent flow regime. They also find applications in different areas like Methanol and FT synthesis, oxidation, and wastewater treatment. However, despite their simple construction and operation, their scale-up is very difficult due to the complex flow fields in these reactors.

We focus on studying the hydrodynamics, mixing, and mass transfer characteristics in bubble columns with internals. The outcome of this work will help provide confident approaches to the scale-up of bubble columns.

Reference: CREL Annual Report 2009-2010 Pages 37 - 44

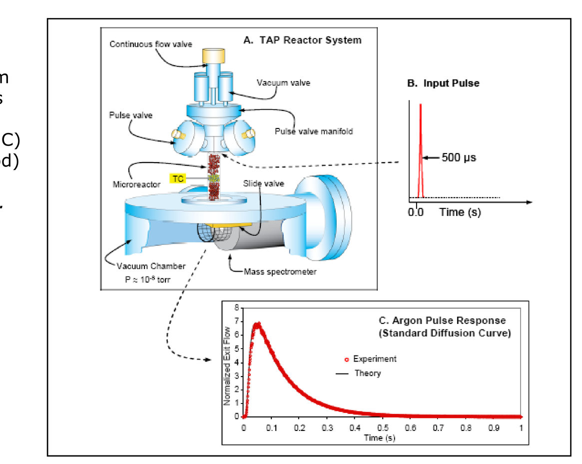
Multiscale Analysis of Methane and Carbon Dioxide Conversion

Vesna Havran

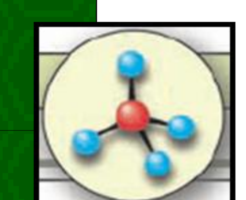
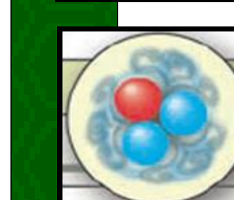
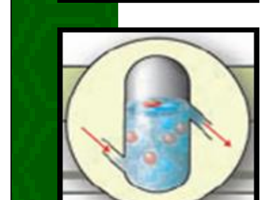


TEM images of different platinum colloidal particles (A) cubic, (B) tetrahedral and (C) star-like (tetrapod) (Lee et al., *Proc. Nat. Acad. of Sci. USA*, 2008)

Methane adsorption on tetrahedral Pt clusters-DFT calculations in CASTEP (Nathan Fine and Cynthia Lo, EECE)



Temporal Analysis of Product (TAP) experimental set up (Gleaves et al., *Catal. Rev. Sci. Eng.*,1988)

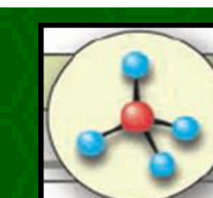
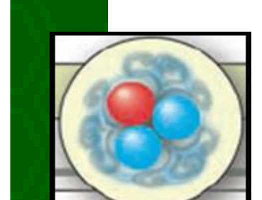
An integrated experimental and computational approach studies CH_4 and CO_2 direct conversion over novel platinum (Pt) nanoclusters of different shapes supported on ceria (CeO_2) that may enhance methane activation. The activity and selectivity of these catalytic nanostructures will be characterized using the temporal analysis of products (TAP) experiment under high vacuum to investigate the nonsteady-state kinetics of the reaction between CO_2 and CH_4.

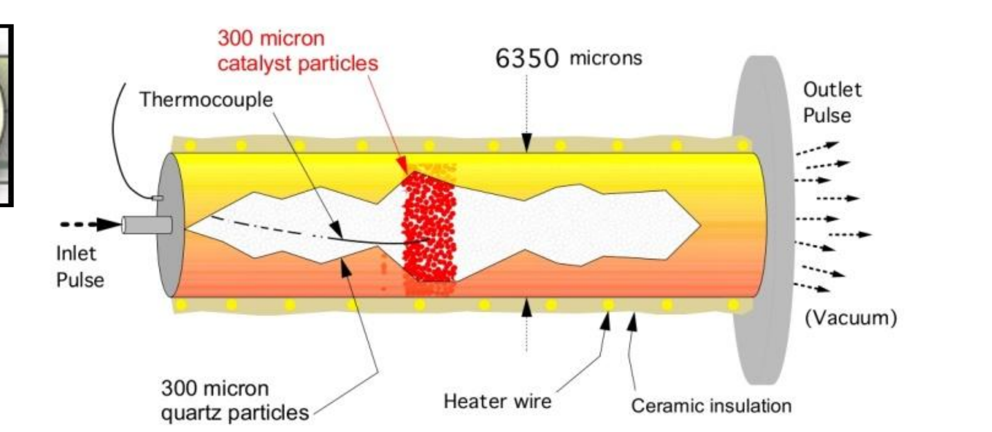
By linking theoretical calculations at the molecular scale with the experimental results obtained from TAP micro-reactor, methodology for the prediction of the lab scale reactor performance will be assessed.

Reference: CREL Annual Report 2009-2010 Pages 69 - 71

Characterization of Catalyst Dynamics with TAP

Evgeniy Redekop



Interrogative, kinetic studies of catalytic materials in TAP Thin Zone experiments provides information for mechanism descriptions, enables the comparison of different catalyst materials and allows for a better understanding of catalyst activity and selectivity as a function of surface coverage.

Current research focuses on the study of CO_2 and CH_4 activation for the conversion of greenhouse gases to useful chemicals.

Reference: CREL Annual Report 2009-2010 Pages 65 - 68