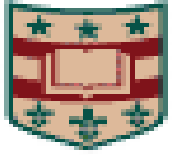


CREL



CREL ANNUAL MEETING, OCTOBER 07
P.A. Ramachandran

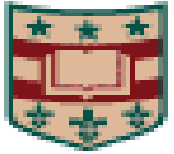
OUTLINE

- General Themes in Modeling
- Specific Current Projects
- Research Opportunities with Industrial Partners

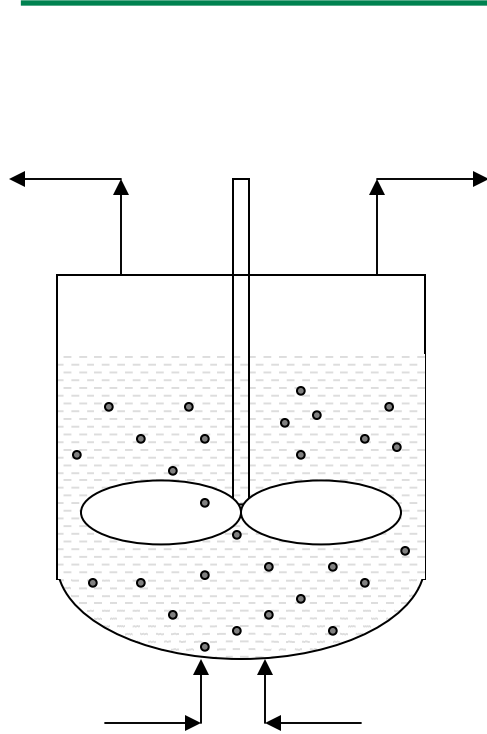
CHEMICAL REACTION ENGINEERING LABORATORY

General Themes

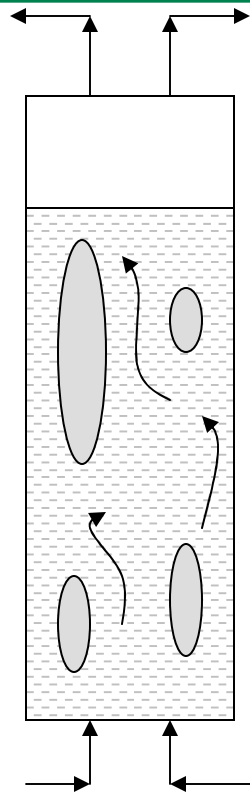
- Multiscale Modeling of Multiphase Catalytic Reactors
- Green Reaction Engineering and Environmentally Beneficial Catalysis
- Process Modeling of semi-conductor and solar grade silicon



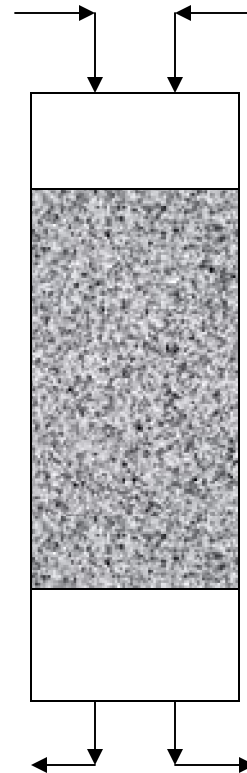
Multiphase Reactors



Slurry Reactor



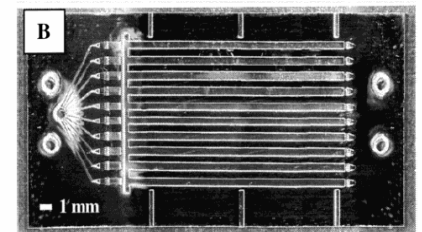
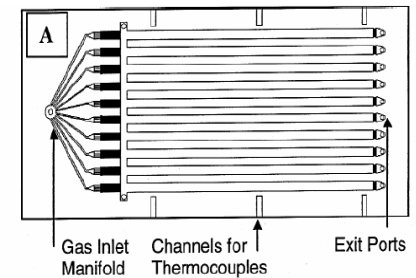
Bubble Column Reactor



Trickle Bed Reactors

Moving Solid Phase

Stationary Solid Phase



Losey et al. (2001)

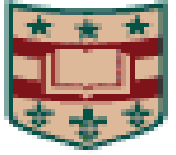
Micro Reactors

Slide 3

SR3

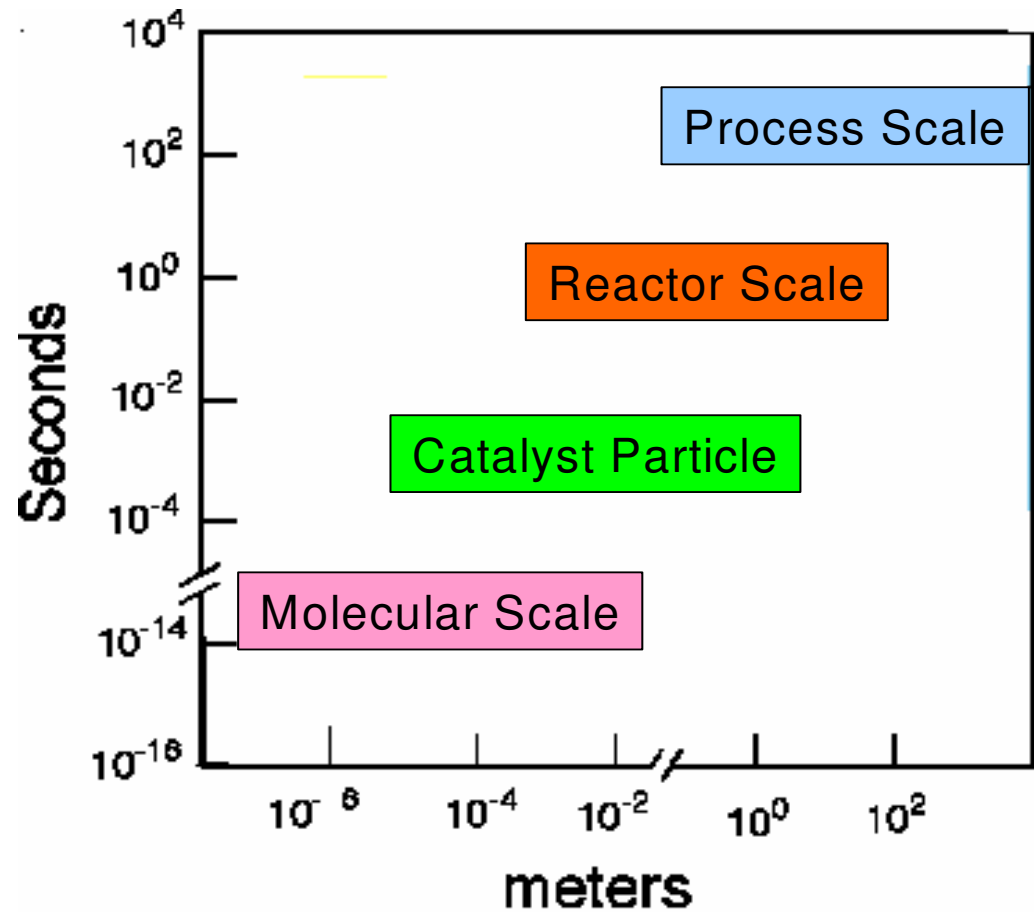
Here the objectives of the project are discribed

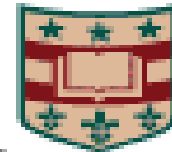
Shaibal Roy, 2/9/2006



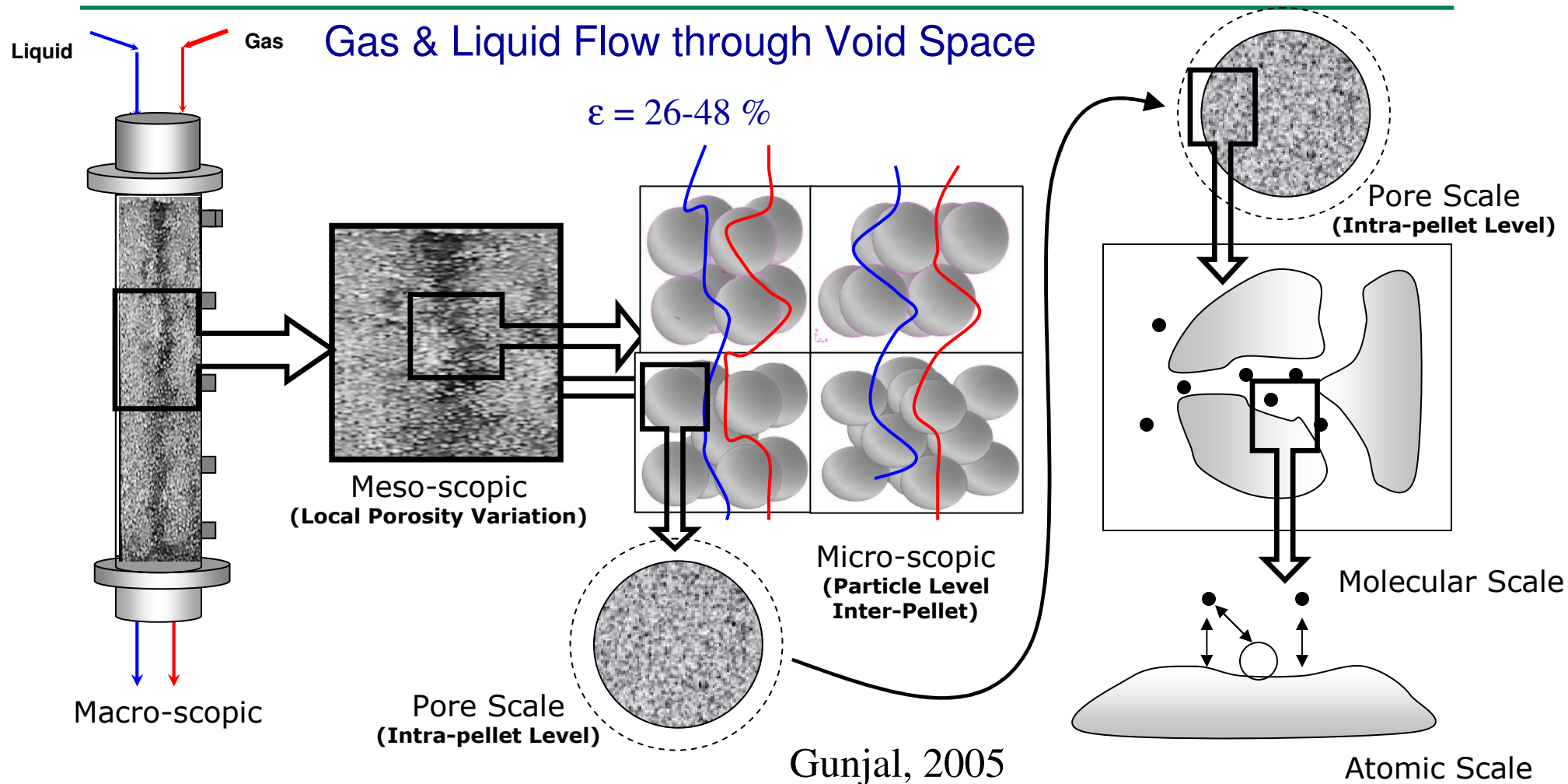
Scales of Modeling

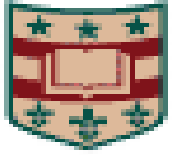
- Molecular
- Micro
- Meso
- Macro
- Plant wide
- Global





Different Scales Involved in the Trickle Bed Reactors



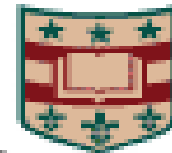


Multiphase flow and Reactor Modeling

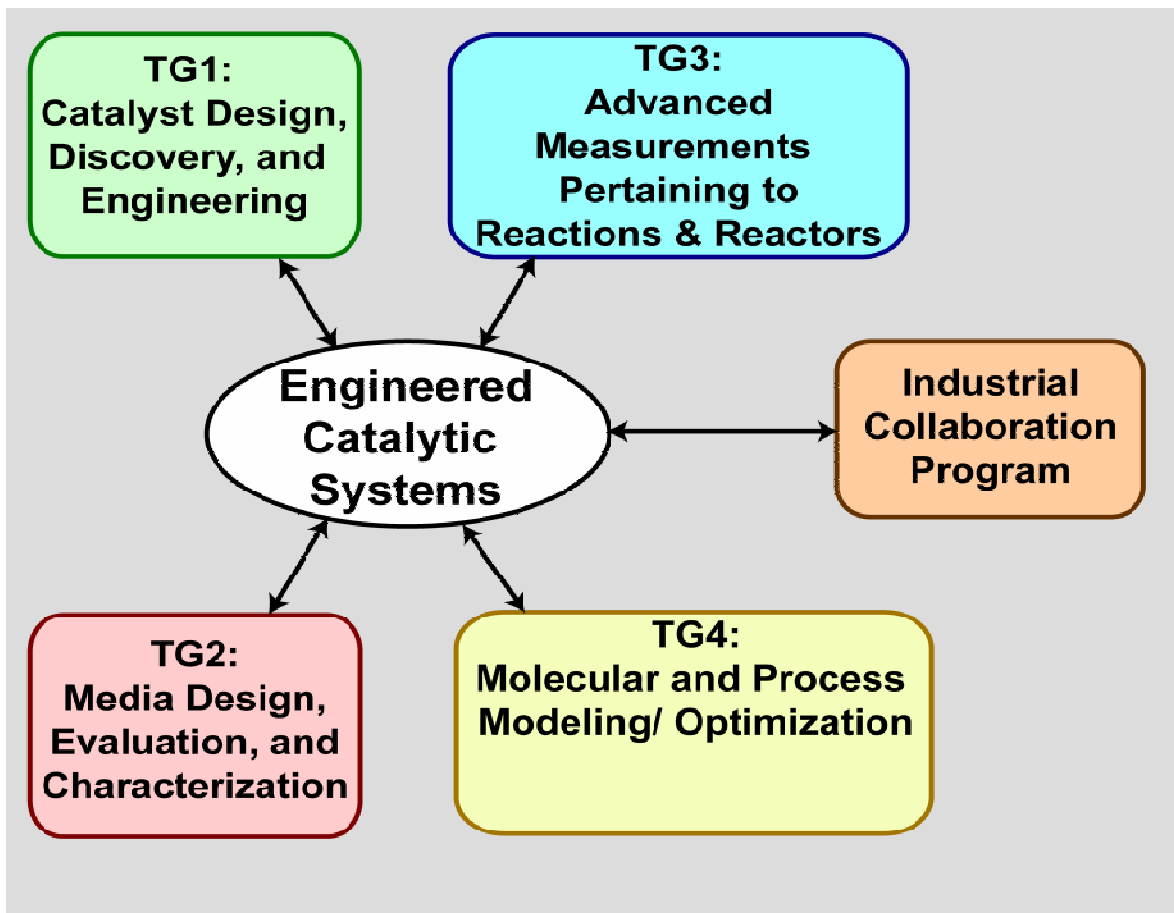
- Trickle Bed Reactors (Combest, Gunjal; CREL group)
 - Trickle Bed Hydrodynamics: Modeling of Hotspot Formation
- Bubble Columns
- Gas-Solid Fluidized Beds (Yue)
- Free interphase Problem (Combest, Gunjal)
- Model Reduction and Novel Computation Techniques

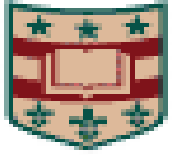
(Evgeniy)

Providing data for hydrodynamic validation is essential before modeling reactive flows ; One of the Focus of CREL Group



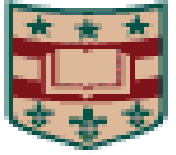
Green Reaction Engineering CEBC





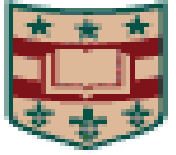
TEST BEDS

- Hydroformylation
- Oxidation
- Acylation
- Alkylation



Hydroformylation

- Hydroformylation of 2-octene in neat and CO₂ media (KU)
- Detailed Kinetic Modeling and Mass Transport Effects (Guha)
- Molecular Models for Metal-Complex Interactions. (KU, RVC)
- Hydrofomylation of other compounds
- Chiral Effects and Selectivity



Oxidation Test Bed: Some Research Objectives

- Large Scale Processes which generate considerable Waste
- Complex Kinetics and Effect of Mass Transfer
- Improvements with higher Oxygen Concentrations (Novel Reactors ?) or (New Solvents?)
- Oxidation of Cyclohexane (Radmilla)

Solid-Acid Catalyzed Alkylation Processes (Nayak)

Environmentally Friendly, Safe & Economical

Technical Challenges

Catalyst Deactivation
Product Selectivity
Reactor Design
Catalyst Regeneration
Product Separation



Multiscale Research Approach

- ❖ Development of multifunctional reactor and catalyst configuration models
- ❖ Transport studies in nanoporous zeolites ([Temporal Analysis of Products, TAP](#))
- ❖ Molecular Dynamics and Grand Canonical Monte Carlo Simulations

Alkylation

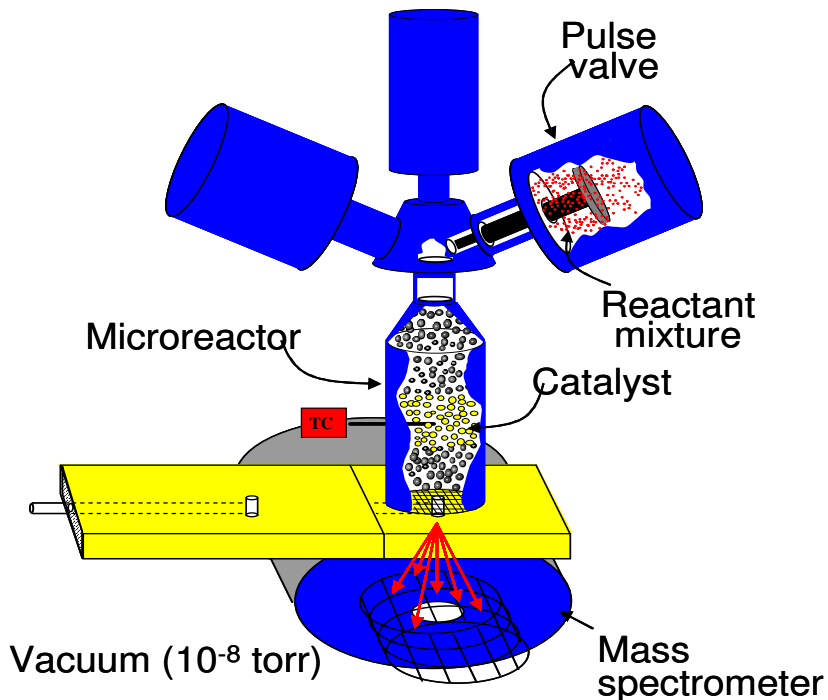
- Butane to Octane (LPG to gasoline)
- Synthetic Detergents (Linear alkylbenzenes)

Trans-Esterification

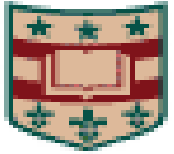
- Biodiesel

Acylation

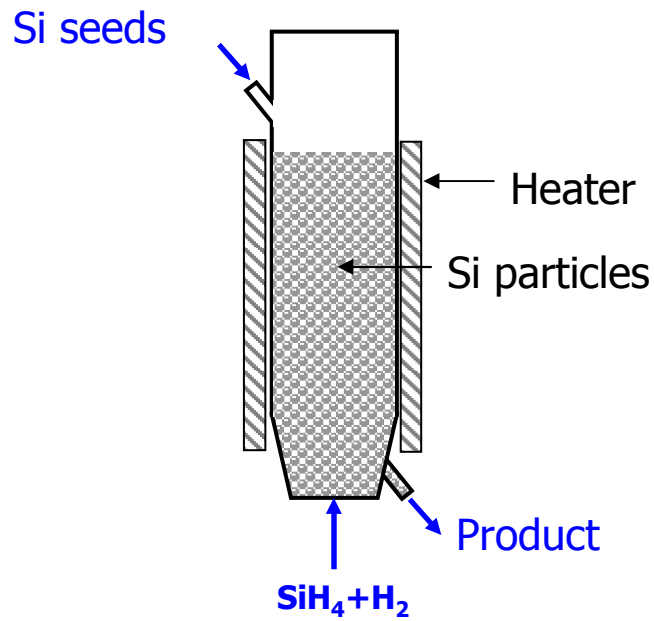
- Methoxybenzene (anisole)
- *2-methoxynaphthalene*
- *i*-butylbenzene (→ First step in Ibuprofen synthesis)



[Temporal Analysis of Product, \(TAP\)](#)

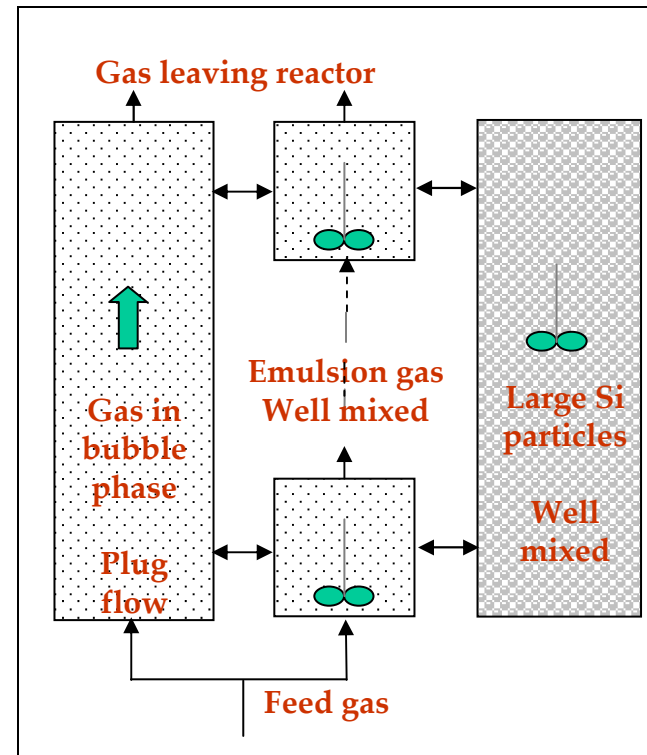


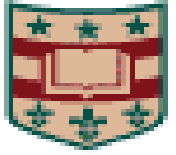
Poly-Silicon Fluidized Bed Process (Yue)



Objective: Maximization of particle growth rate

Reactor Model

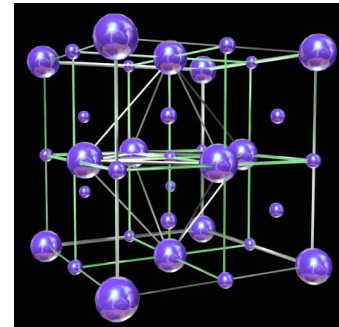




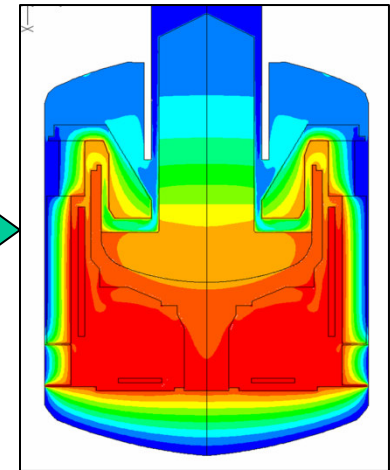
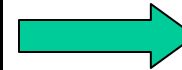
Mono-Silicon CZ Crystal Growth (Gunjal)



Czochralski Crystal Growth Process

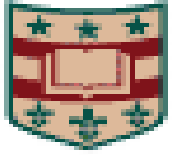


Atomic Rearrangement of Si-Crystals



Computational Model for Cz-Crystal Growth Process

Objective is tight control of Silicon crystal quality at maximum growth rate and minimization of defects and dislocations



Collaboration Opportunities

- CFD Modeling; Meso-Scale CFD and Improved Closures, Non-isothermal Effects.
- Comprehensive Models of Trickle Bed Reactors
- Model Reduction Methods and Improved Phenomenological Methods
- Adsorption-Diffusion in Zeolites and Solid Acids
- Stirred and Micro-reactors for Kinetic Measurements