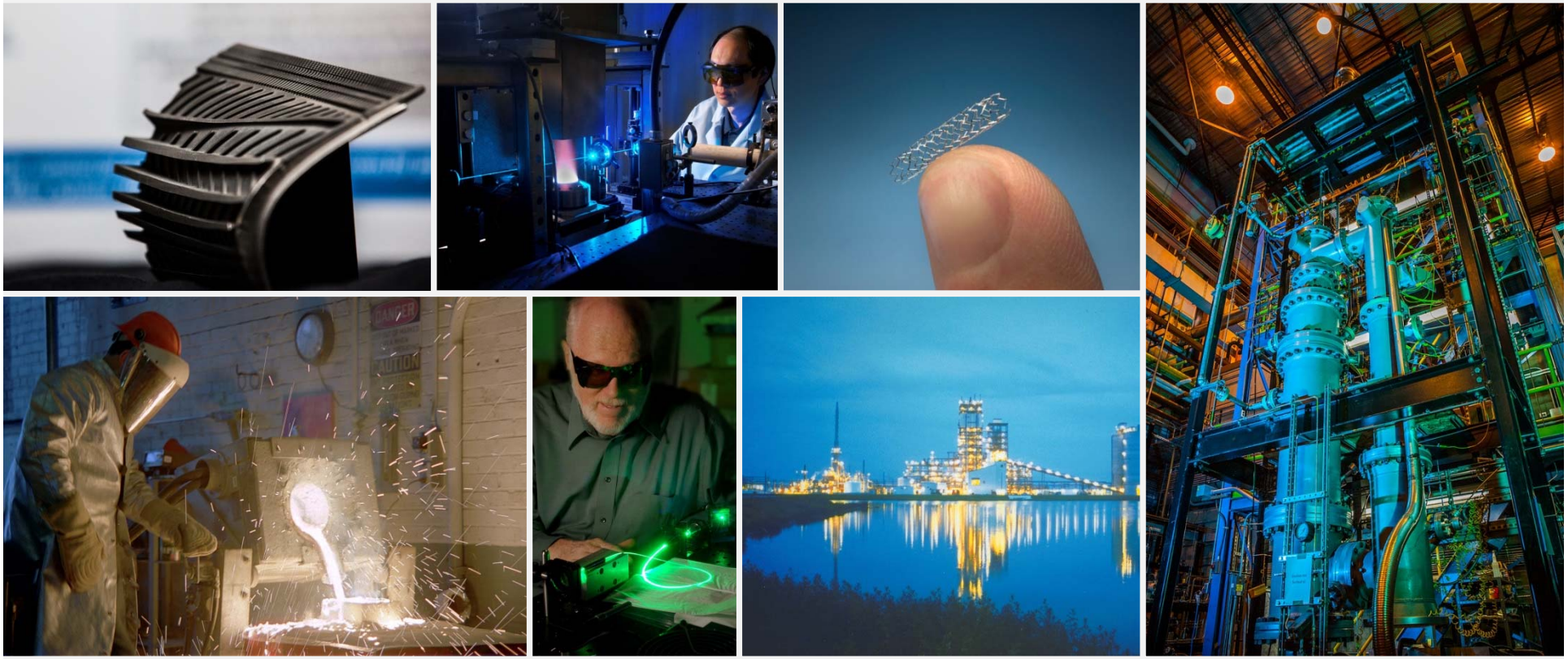
Driving Innovation ♦ Delivering Results



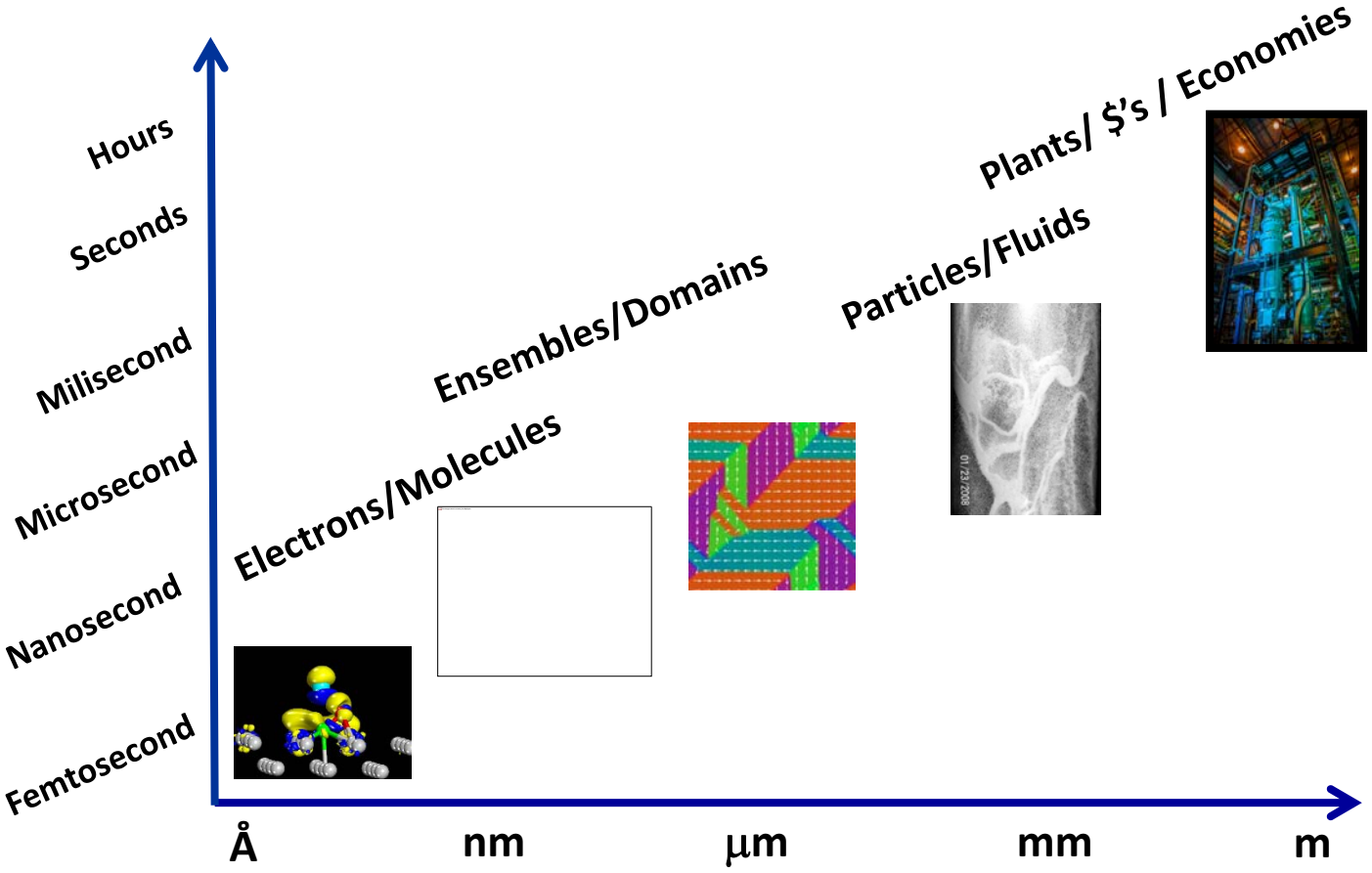
Radically Engineered Modular Systems (REMS)

Research Team: Christopher Matranga, James Bennett, Ronald Breault, William Rogers, Dushyant Shekhawat

Management Team: Geo Richards, David Alman, Madhava Syamlal, Jenny Tennant

U.S. DEPARTMENT OF ENERGY | National Energy Technology Laboratory

Reaction Chemistry & Engineering Occurs at ALL Scales



Transformational Energy Technologies Require Input & Mastery at ALL Levels

REMS Will Reduce Time, Cost, and Risk

Gasification Challenges:

- New approaches for coal to power/chemicals technologies $$$$ to develop & deploy
- Capital costs for plant ($$$$)
- Varying feedstocks, distributed power generation

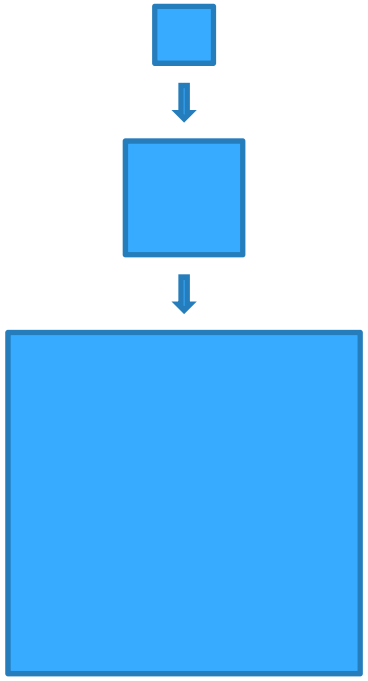
How do we address?:

- Reduce time/risk scale up
- Reduce build/capital costs
- Fuel flexible designs, distributed systems
- Enhanced reactor/process performance
  - *Reaction manipulation at the particle level*

CFD led Reactor Design, Advanced Manufacturing, & Reaction Intensification offer unique opportunities to address these challenges

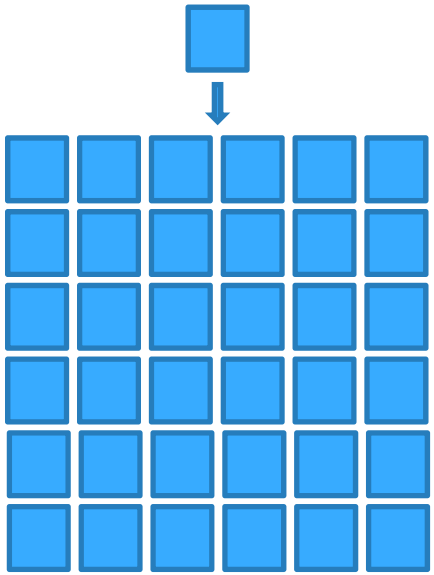
How Will REMS Differ from Traditional Approaches

Traditional



- Unreliable scale up
- Expensive, long development
- Incremental improvements

REMS



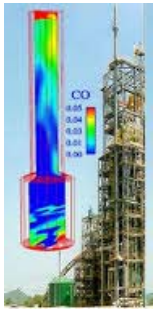
Beat economies-of-scale by using

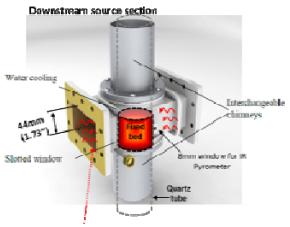
- CFD to rapidly create novel reactor configurations
- Microwave, plasma etc. to intensify reactions
- Advanced manufacturing to replicate reactors at low cost

Example of Emerging Industrial Approach

Velocys: Small, Modular & Efficient GTL Reactors

Radically Engineered Modular Systems (REMS): Research Areas



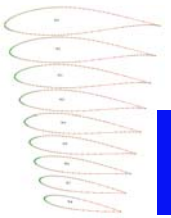


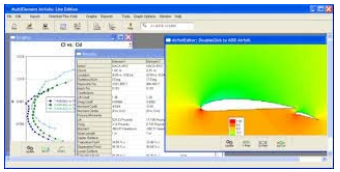
- **CFD-led reactor & process design (Bill Rodgers)**
  - Development of physics-based submodels
  - CFD Optimization and Toolsets
- **Reactor Characterization and CFD Model Validation (Ron Breault)**
  - 3D printing for rapid testing
  - Development of characterization tools
- **Advanced Manufacturing and Reactor Materials Development (James Bennett)**
  - Materials for unusual reactor geometries & conditions
  - Rapid, cheap, fabrication techniques
- **Reaction Intensification (Dushyant Shekhawat)**
  - Microwave/Plasma driven reactors
  - Catalyst Design

Radically Engineered Modular Systems (REMS)

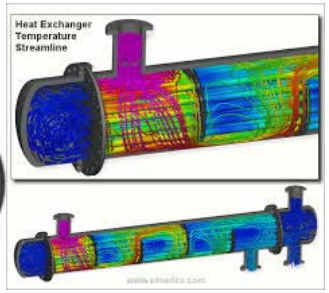
Use CFD Simulation-Based Optimization for Reactor Design

Build on Existing Techniques

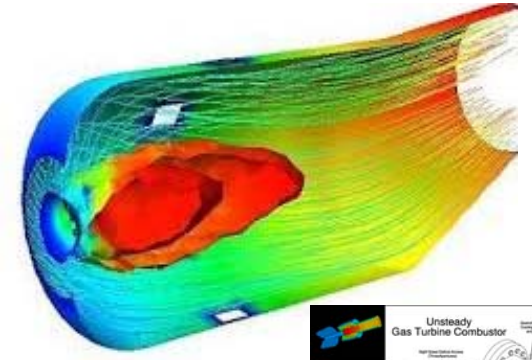


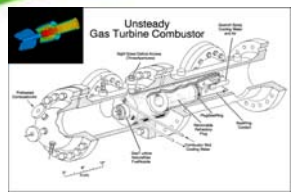


- **Use of CFD-Based Optimization is growing for single phase applications**
  - Proven technique in many engineering applications - chemical process, aerospace, turbomachinery, automotive
    - Optimization of airfoil shape for lift and drag
    - Optimization of heat exchanger tube shape, size, location
    - Optimal combustor design



- **REMS will develop, validate, and apply a <u>Multiphase CFD-based Optimization Toolset</u>**
  - Multiphase CFD brings new challenges to the optimization process
    - Complex multiphase physics require accurate submodels for flow, heat transfer, chemical kinetics, coupling between phases
    - Very computationally intensive
    - Potential for huge datasets resulting from pilot and industrial scale applications
  - The new software capability will be based on the NETL **MFiX Suite** of multiphase flow CFD software



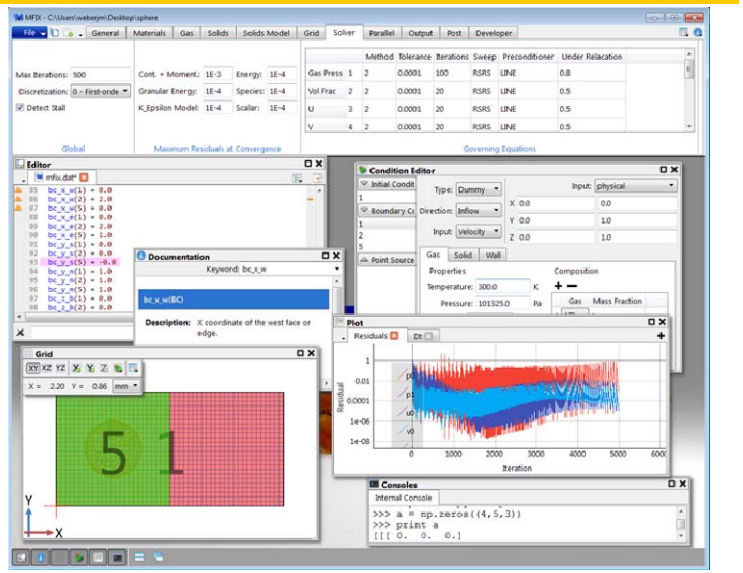


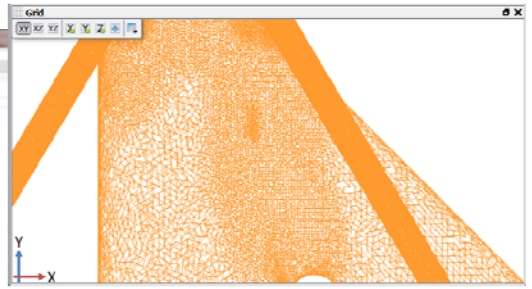
Radically Engineered Modular Systems (REMS)

Use CFD Simulation-Based Optimization for Reactor Design

User Interface and Toolset to Manage the Optimization Process

- **Design and develop GUI-based, Multi-objective Optimization software framework**
  - Code infrastructure for managing the optimization process
  - methodologies and code to create and manage reactor models created using MFIX Suite of multiphase flow software
- **The modeling tools will become part of the publicly available, Open Source MFIX Suite of codes (https://mfix.netl.doe.gov)**



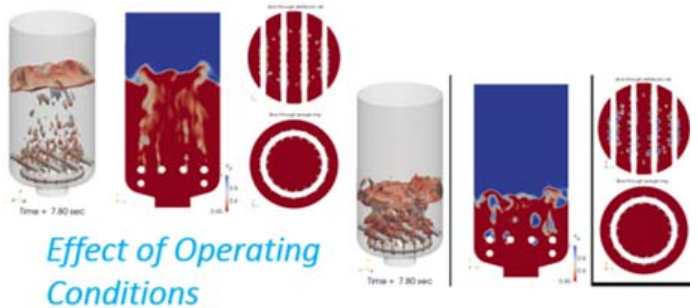


Radically Engineered Modular Systems (REMS)

Use CFD Simulation-Based Optimization for Reactor Design

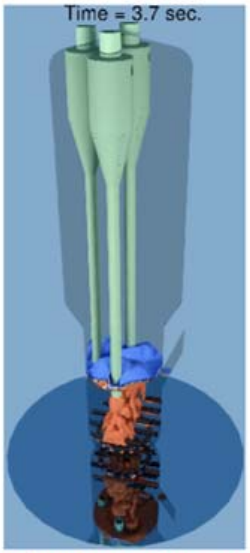
Use CFD Simulation-Based Optimization for Reactor Design

- **Optimization process will investigate radically different reactor geometries**
  - Allow for precise manipulation of different coal and biomass particles
    - segregation of low ash melting particles in a lower temperature part of the reactor
    - continuous removal of ash or volatiles as they are created,
    - segregation of char to a higher temperature part of the reactor
    - segregation of catalysts and reactive particles types for more efficient conversion
    - use of neutral/reactive particle addition and removal
  - Optimize reactant and product gas flow
    - improve particle-gas contacting to better control carbon conversion and product composition
    - Control heat addition/removal, etc.



Effect of Operating Conditions

Geometry Changes



Scale Up Performance

Advanced Reactor Characterization: 3D Printing of CFD designed reactors

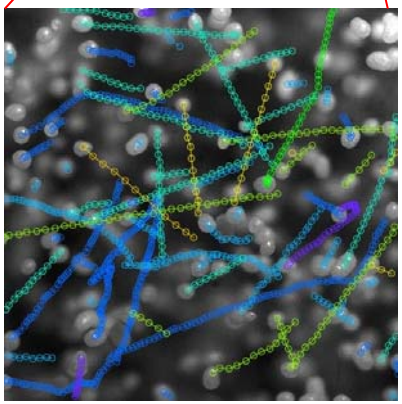
CAD Design of gas-liquid contactor

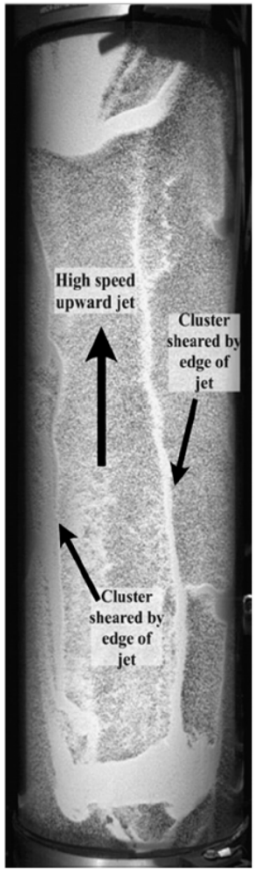
Printed & Assembled Contactor

CFD simulation Of gas flow

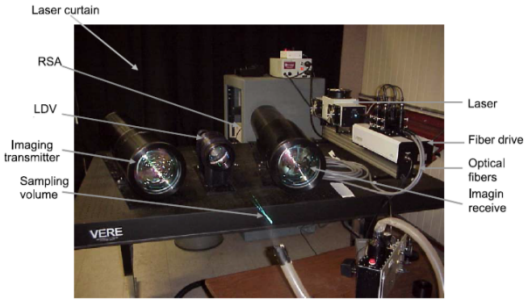
Advanced Reactor Characterization: Validating & Improving CFD Models

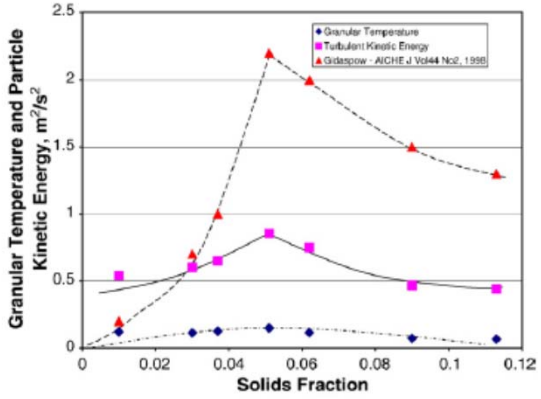
High Speed Particle Imaging & Flow Characterization



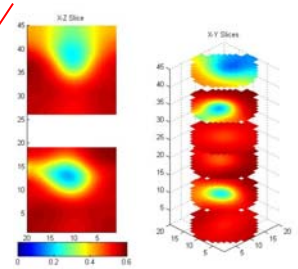


Laser Doppler Velocimetry

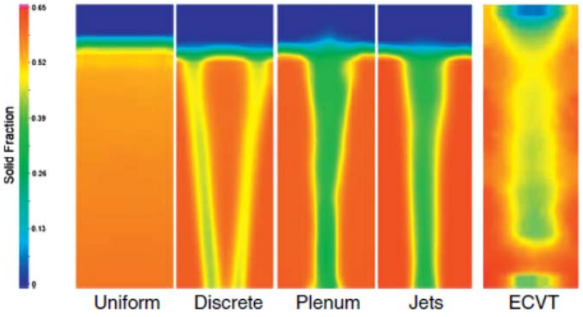




Electro Capacitance Volume Tomography (ECVT)

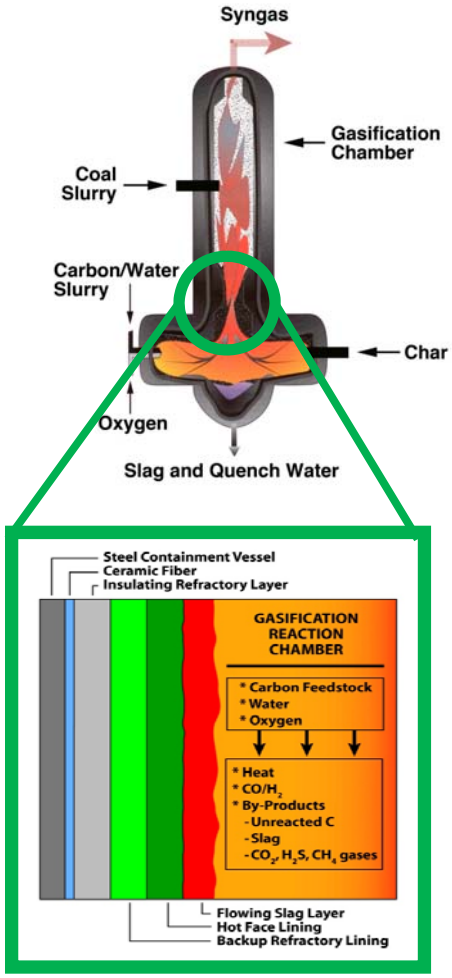


CFD Models Exp

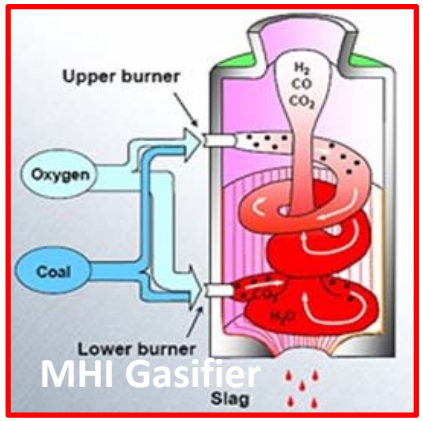


Advanced Manufacturing: Making REMS a Reality

"Traditional"



REMS



HOT!!

Ceramic
8 mm

Bonding
100 microns

Metal
8 mm

Cold

- Brick lined reactors unsuitable for unusual geometries
- T, P, & Flow Fields require differing materials in reactor zones
- Subtle variation of reactor size & characteristics for varying feedstocks requires variations of materials used

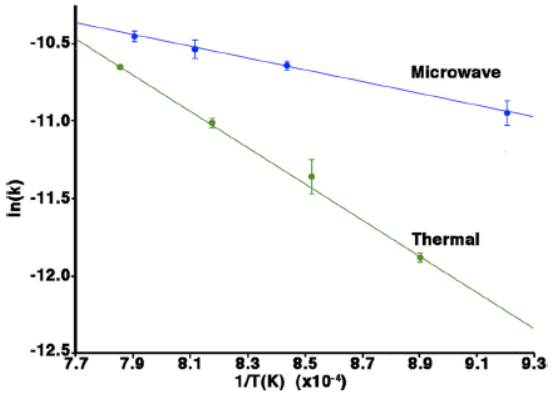
Few methods exist to manufacture reactors with these properties

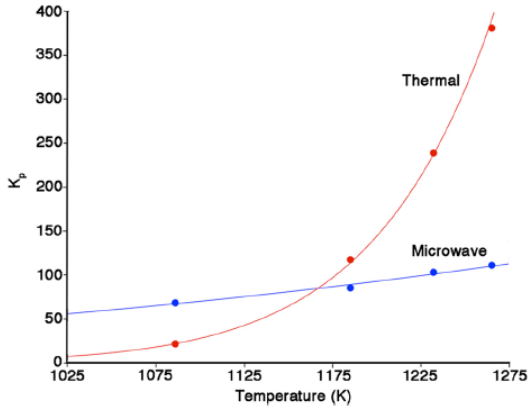
Reaction & Process Intensification: Non-traditional Energy sources

Microwave Enhanced Boudouard Reaction

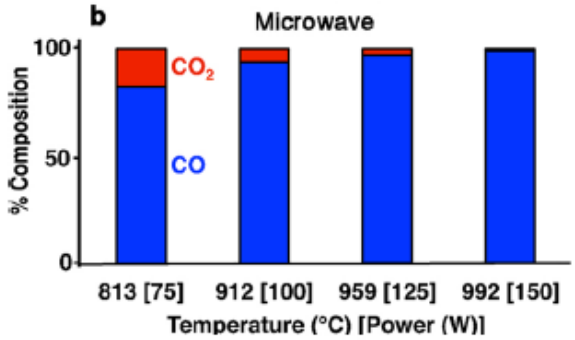
$$C + CO_2 \rightleftharpoons 2CO \qquad \Delta H = 172\ kJ/mol$$

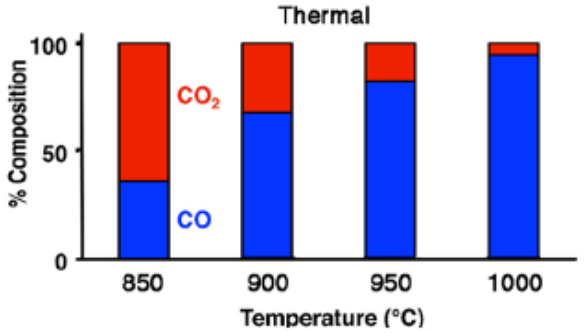
Altered kinetics & equilibrium constants





Altered product distributions



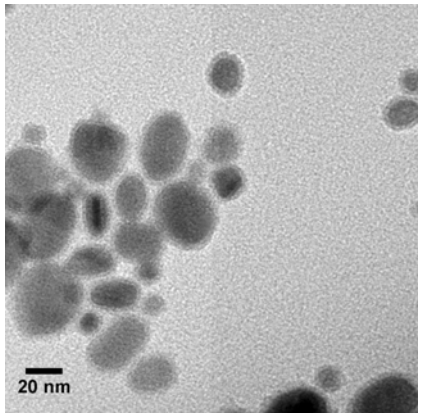


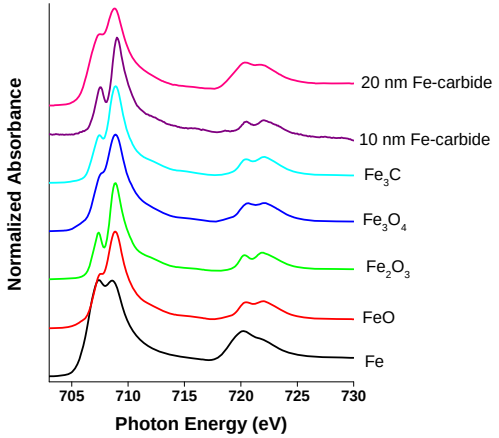
- MWs, plasmas, etc deposit energy in "non-thermal" manner
- Product streams deviate from thermodynamic predictions & traditional thermal reactors
- Cost of energy source has to be weighed against process benefits

Figures from Stiegman et. al. J. Phys Chem C 117, 2013, pgs 26871-26880

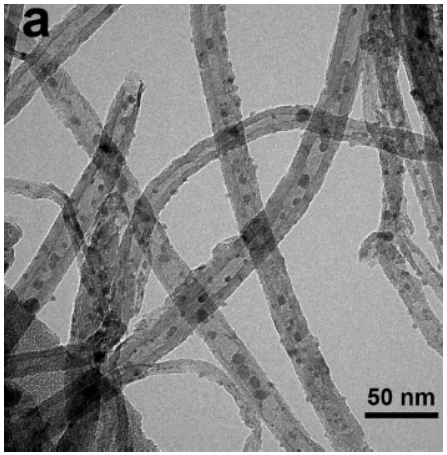
Reaction & Process Intensification: Catalyst Design & Engineering

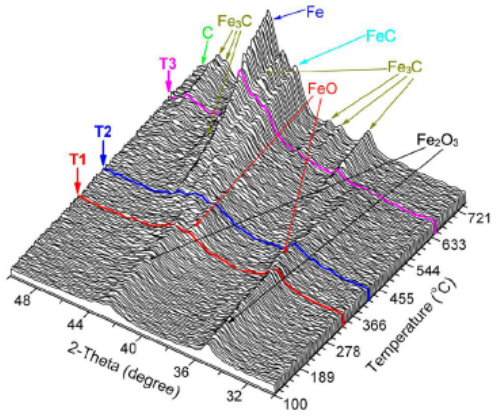
Nano-Fe_5C_2





Fe inside of Carbon Nanotubes





- Encapsulation in CNTs improves Fe active phase stability for FT rxns
- Nano Fe-carbides are now possible in high yield
- Possible to design & optimize materials specifically for use with microwaves sources etc

It's All About a Clean, Affordable Energy Future




For More Information, Contact NETL

the ENERGY lab

Delivering Yesterday and Preparing for Tomorrow