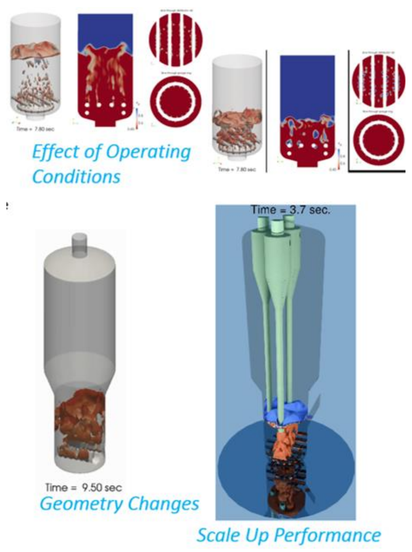
Using Multiphase CFD Simulation-Based Optimization for Coal Reactor Design

Radically Engineered Modular Systems (REMS)

Use CFD Simulation-Based Optimization for Reactor Design

Use CFD Simulation-Based Optimization for Reactor Design

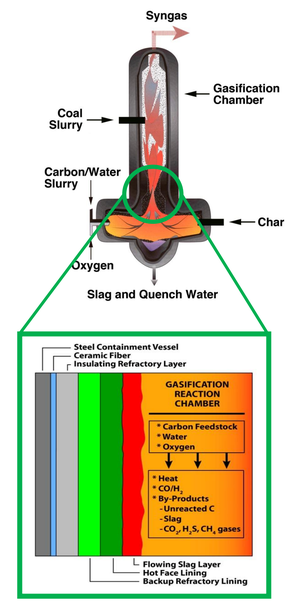
- **Optimization process will investigate radically different reactor geometries**
  - Allow for precise manipulation of different coal and biomass particles
    - segregation of low ash melting particles in a lower temperature part of the reactor
    - continuous removal of ash or volatiles as they are created,
    - segregation of catalysts and reactive particles types for more efficient conversion
    - segregation of char to a higher temperature part of the reactor
    - 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.



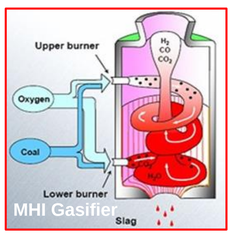
- Technical Lead & Contact: Bill Rogers; William.rogers@netl.doe.gov

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

- Technical Lead & Contact: James Bennett, james.bennett@netl.doe.gov

Advanced Reactor Characterization: 3D Printing of CFD designed reactors

CAD Design of gas-liquid contactor

Printed & Assembled Contactor

CFD simulation Of gas flow

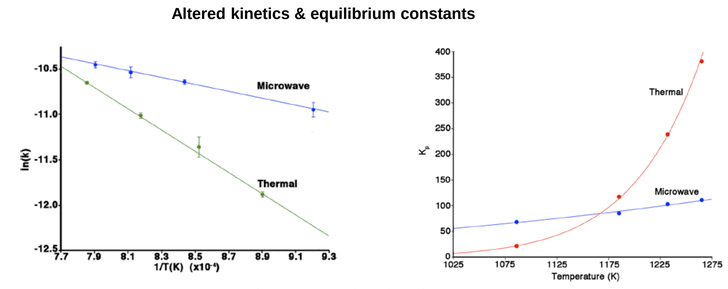
- Image from J Bara et. al. Nanomaterials and Energy 2013

Reaction & Process Intensification: Non-traditional Energy sources

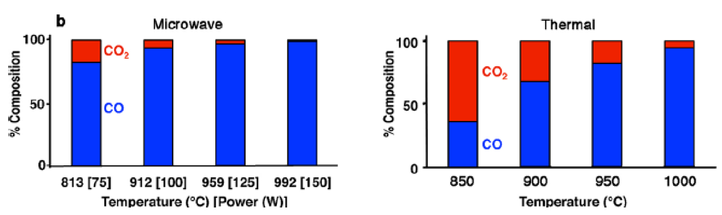
Microwave Enhanced Boudouard Reaction

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

Altered kinetics & equilibrium constants



Altered product distributions

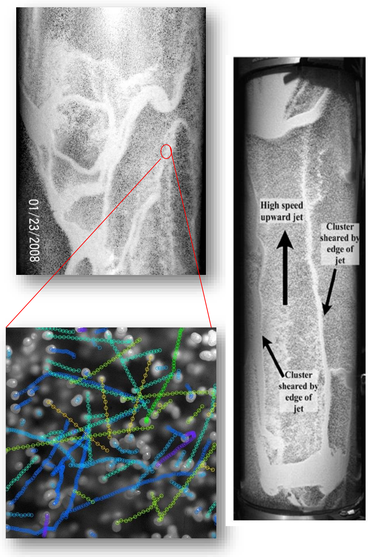


- MWs, plasmas, etc deposit energy in "non-thermal" manner
- Product streams deviate from thermodynamic predictions & traditional thermal reactors
- Cost of energy source has to be weighed against process benefits

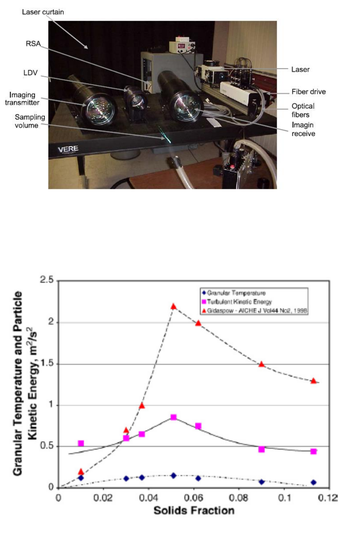
- Figures from Stiegman et. al. J. Phys Chem C 117, 2013, pgs 26871-26880

Advanced Reactor Characterization: Validating & Improving CFD Models

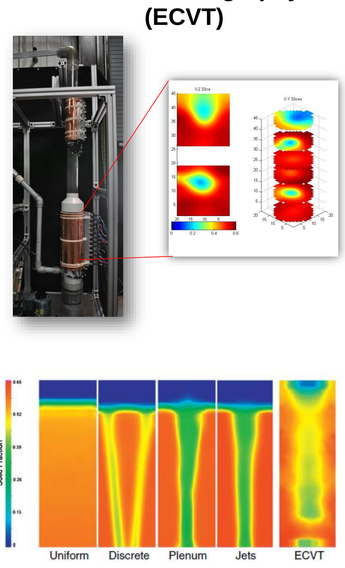
High Speed Particle Imaging & Flow Characterization



Laser Doppler Velocimetry



Electro Capacitance Volume Tomography (ECVT)



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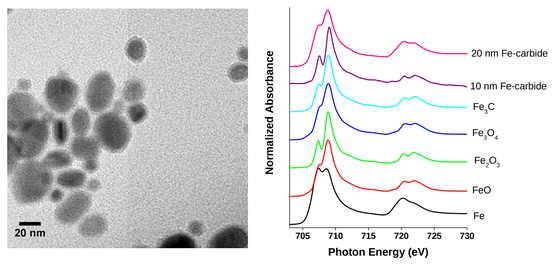
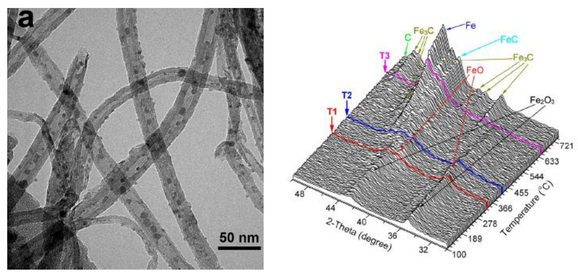
Reaction & Process Intensification: Catalyst Design & Engineering

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

Top: NETL Results; Bottom: Bao et. al. JACS