Modeling of Black Liquor Gasification in a Bubbling Fluidized Bed

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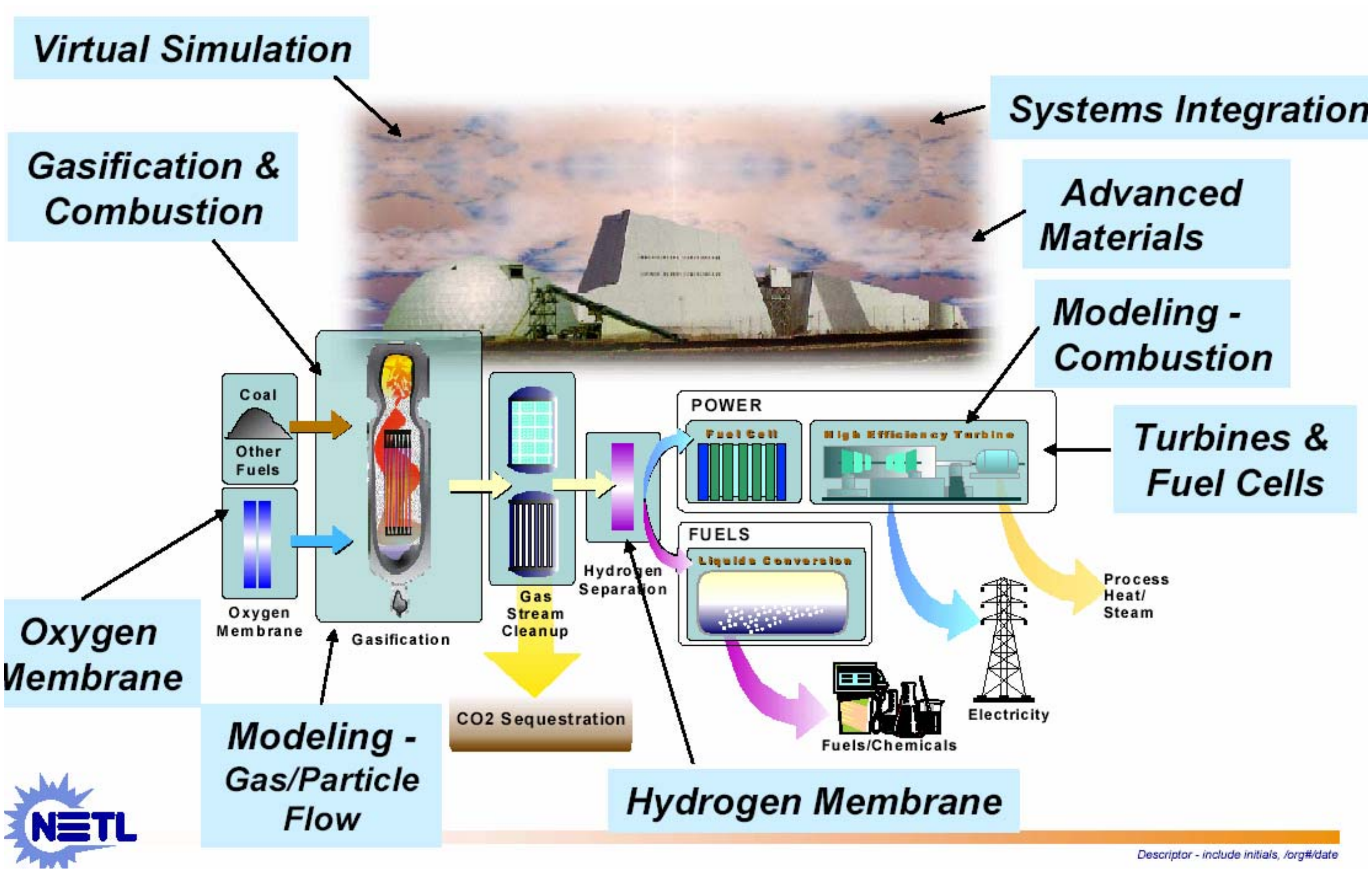
Biomass Utilization Workshop
February 10, 2004

Gasification of Solid Fuels



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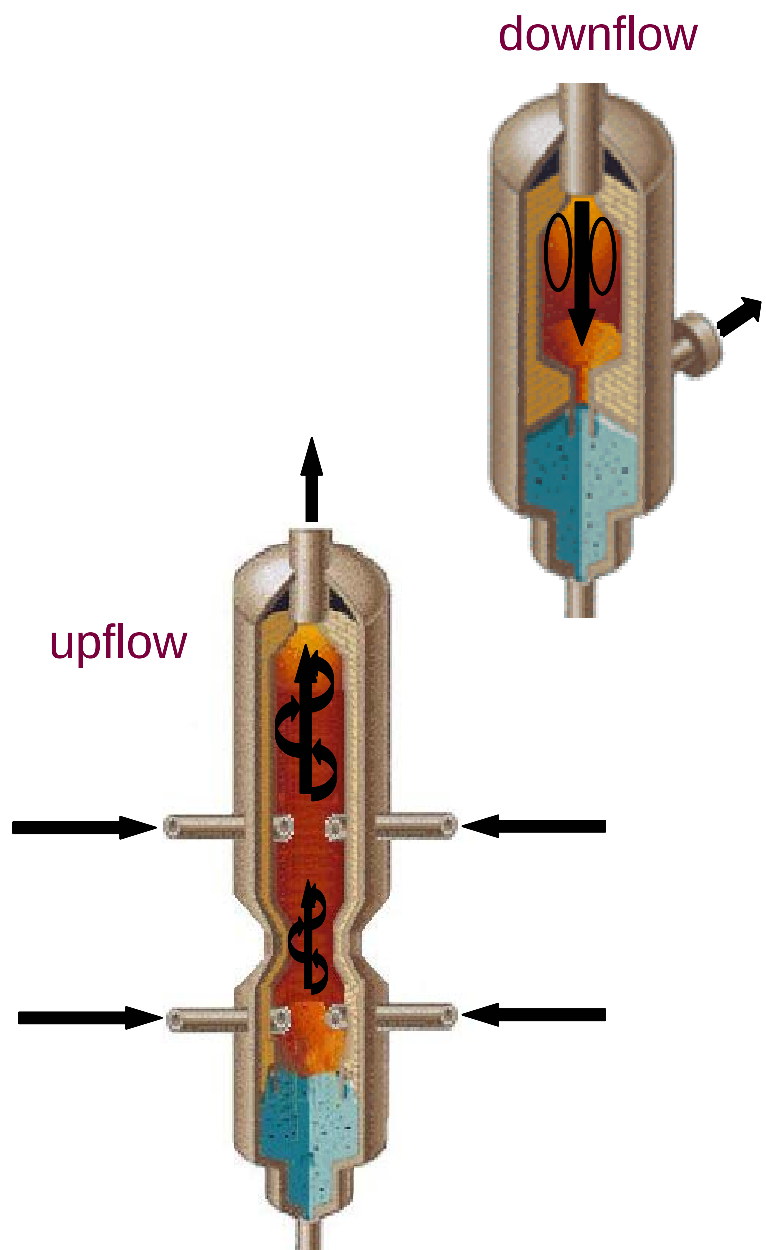
Entrained Flow Gasifier Model

- **Model Development**
  - **Configurations:**
    - **downflow / upflow**
    - **1 stage / 2 stage**
    - **based on public information**
  - **Parameters**
    - **Process conditions, burner characteristics**
    - **Fuel type, slurry composition**
    - **gross geometry**
  - **Submodel developments**
    - **high pressure gasification reaction kinetics**
    - **slag, ash, soot, tar**
    - **air toxics (metals, PM2.5)**
- **Collaborations**
  - **EPRI**
  - **Black Coal CCSD, Australia**
  - **IVD, U. of Stuttgart**

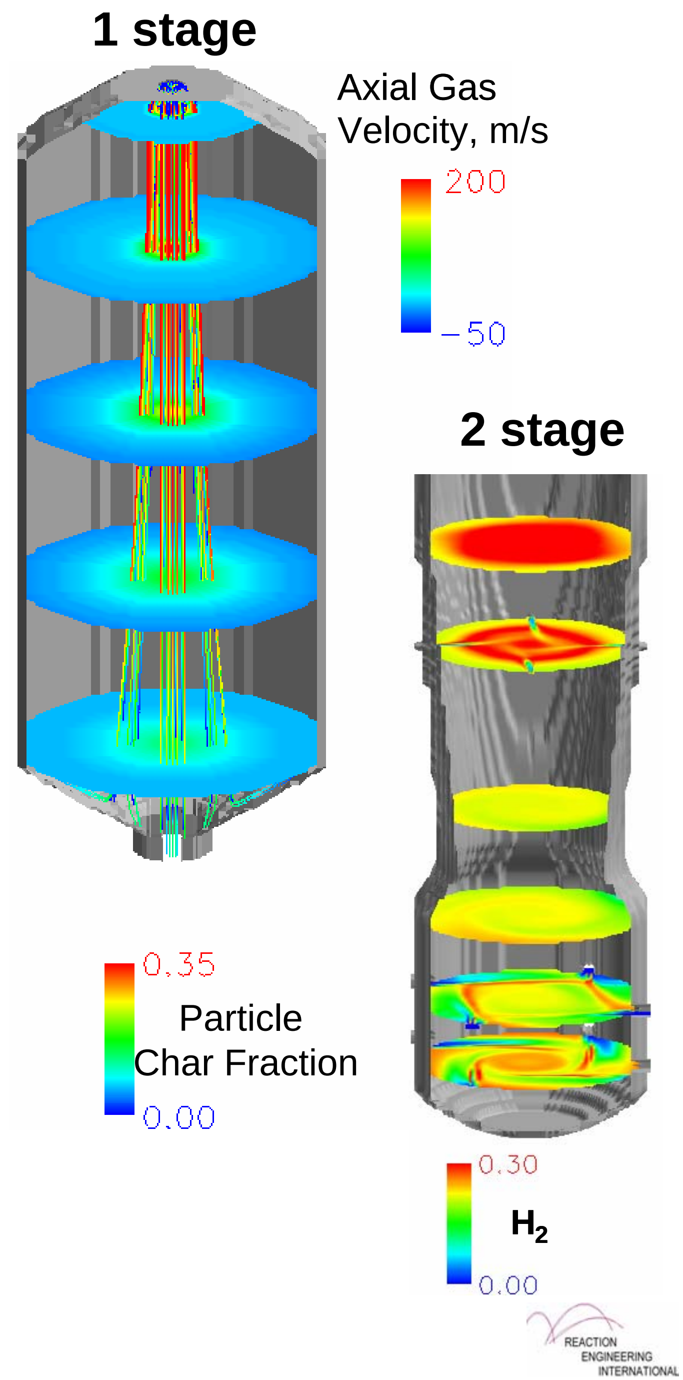


Gasifier - CFD Model

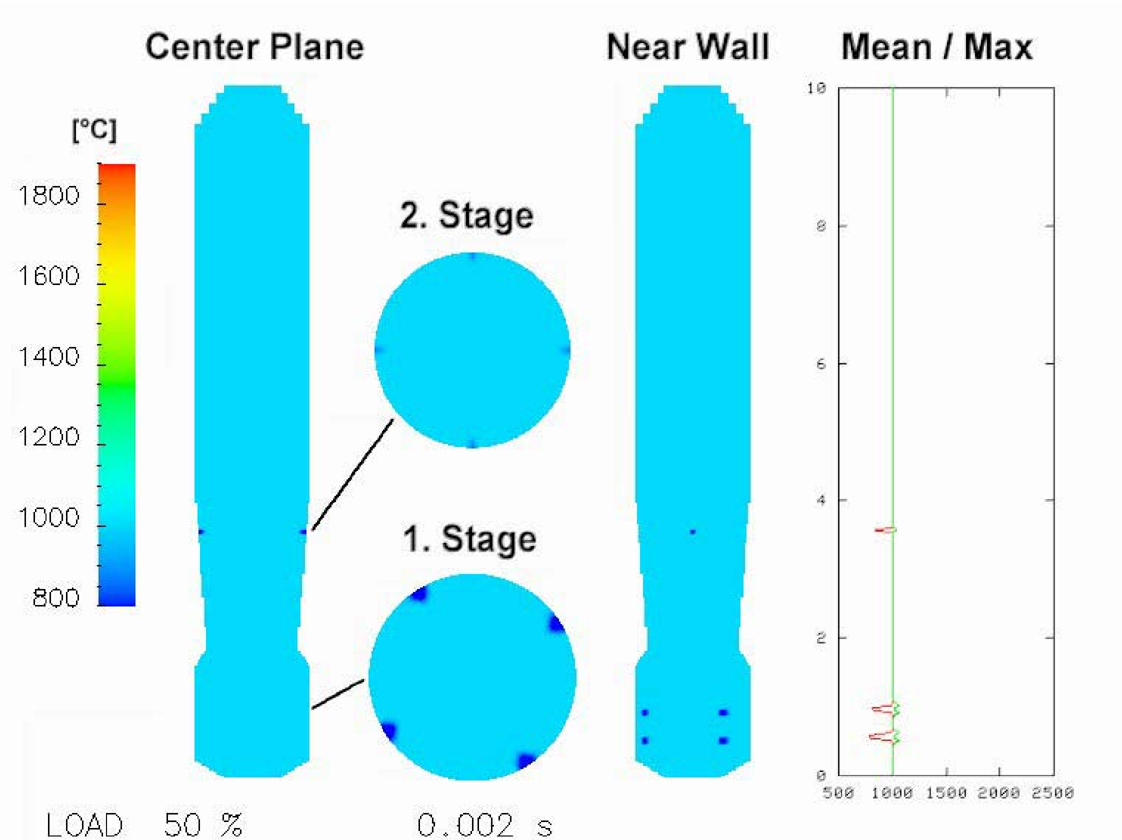
- **1 & 2 stage gasifier designs**
- **provides details on**
  - **gas flow field**
    - » temperature, velocity, species
  - **wall conditions:**
    - » temperature, heat flux
    - » critical viscosity, slag flow
  - **carbon conversion, cold gas efficiency**
  - **unburned carbon in slag and flyash**
  - **generated syngas**
    - » speciation, temperature, particle loading,...
- **evaluate impact on**
  - **carbon conversion, syngas, slag and ash properties, refractory**

due to:

- **fuel change or co-firing:**
  - » coal / char-recycle / petcoke / waste / biomass
- **oxidant: oxygen concentration, pre-heat**
- **feed: wet vs dry, solids loading, pre-heat**

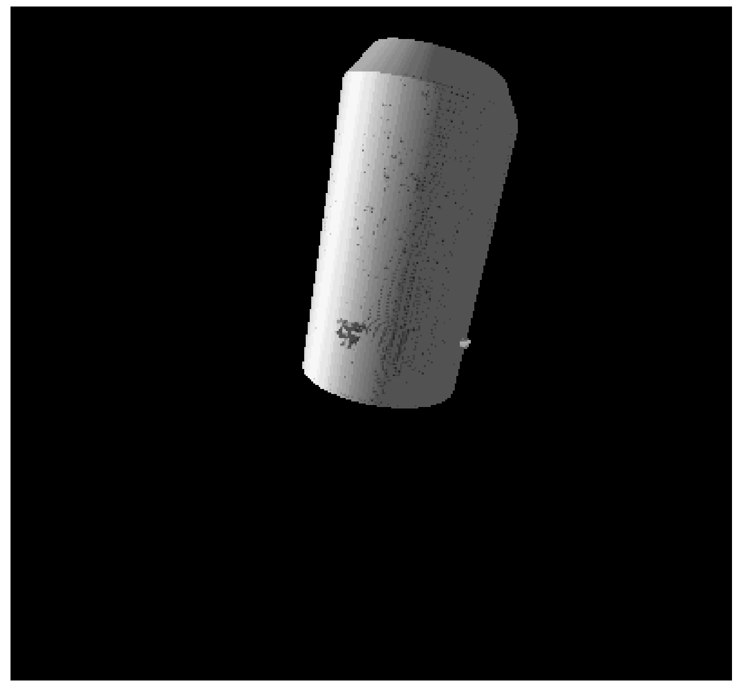


Detailed Results



liquid slag thickness

mm
8
0

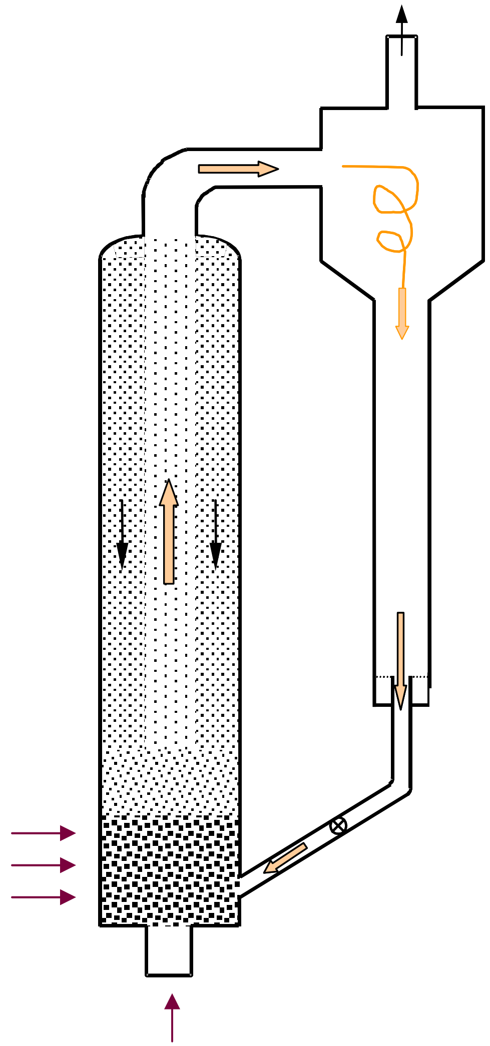


Gasifier – Transport Reactor

- 1.5D, CFB, core/annulus engineering model
- Provides elevation profiles for
  - gas flow field
    - » temperature, velocity, species
  - wall conditions
    - » temperature, heat flux
  - solids
    - » carbon conversion, particle size
    - » coal, char, limestone, sand
- Overall estimates for
  - cold gas efficiency
  - syngas: speciation, temperature, particle loading
  - solids/particles: size distribution, carbon conversion
- evaluate impact on
  - carbon conversion, syngas quality, particle size, refractory

due to:

- fuels: coal / petcoke / waste / biomass / char
- oxidizer: air, oxygen blown/enriched, pre-heat
- FGR
- solids: grind, drying, pre-heat



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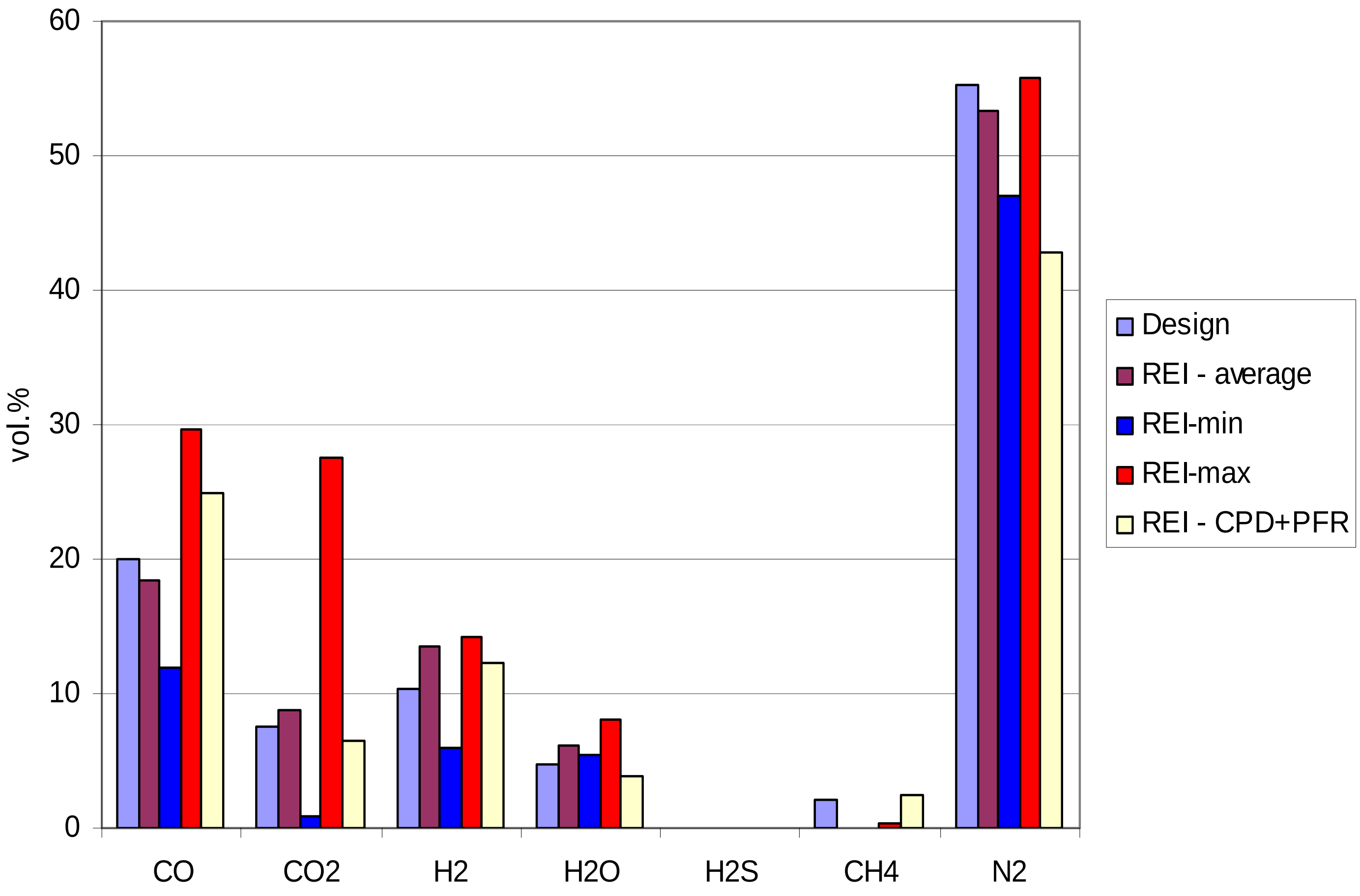
Syngas Composition Predictions

Fuel type	Powder River Basin, Alabama Calumet Bituminous
Fuel particle size, µm	200 - 350
Fuel feed rate, pph	2700 - 5000
Sorbent type	Ohio Bucyrus limestone
Sorbent particle size, µm	10 - 30
Sorbent feed rate, pph	0 - 200
Reactor temperature, °F	1670 - 1825
Reactor pressure, psig	140 - 240
Riser gas velocity, fps	40 - 60
Riser mass flux, lb/ft^{2}s	150 - 700
Air/coal mass ratio	2.5 - 3.5
Steam/coal mass ratio	0.0 - 1.0



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Fluidized Bed Gasification of Black Liquor

- **A key DOE/Georgia Pacific supported technology option (MTCI) being demonstrated at Big Island, VA**
- **Features:**
  - bubbling bed
  - high efficiency & chemical recovery
  - improved emissions
  - lower maintenance costs
  - elimination of smelt/water explosion hazard
- **Modeling Objectives:**
  - describe impact of design conditions and operating conditions
  - support troubleshooting with pilot and demonstration units

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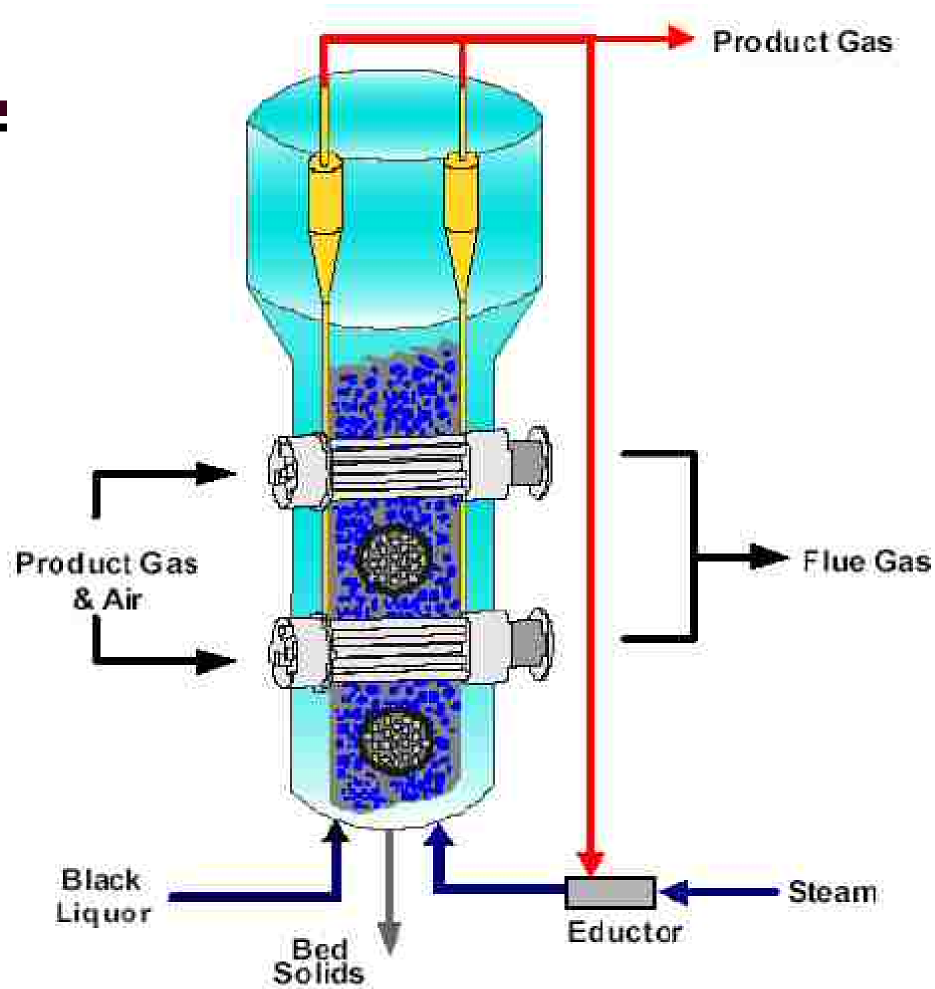
MTCI Specifics

- Steam reforming process operating in the bubbling regime
- Design capacity of 180 tons/day
- Design incorporates 4 tube bundles (pulse combustors) with 253 horizontal tubes each, arranged in a staggered configuration



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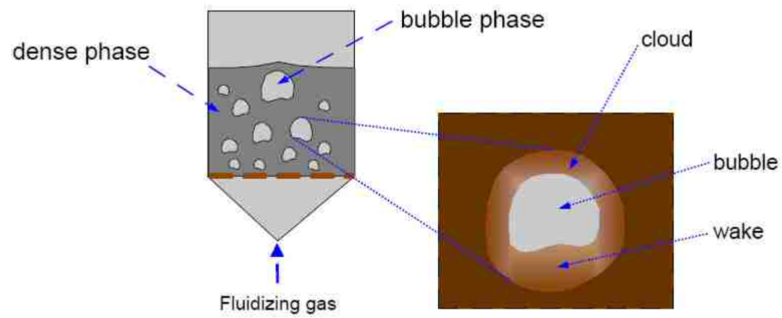
Model Approach



- **Three phase counter-current with back mixing**
  - **particle free bubble phase**
  - **wake-cloud phase**
  - **dense particle phase**
- **Gas in different phases at same temperature**
- **Particle temperatures in different phases are treated separately**
- **Bubble size and velocity determined using standard correlations such that:**
  - **bubbles grow with height**
  - **bubbles break up in tube banks**
- **Bubbles play a major role in driving solids circulation in bed impacting temperature distribution, concentration profiles, and bed agglomeration**

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Particle Models

Devolatilization

- Empirical correlations are used to determine C, H, O and S release (Frederick and Hupa, 1993; Frederick et al., 1995)
- Volatiles are represented by a mixture of CH_4, CO, H_2O and H_2S

$$C_aH_bO_cS_d = eCH_4 + fCO + gH_2O + hH_2S$$

- Amount of each gas species released is determined from the element mass balance

Gasification Kinetics

- Steam gasification (Li and van Heiningen, 1991; Wessel et al., 1997)

$$C + H_2O = CO + H_2 \qquad \text{Rate} = 2.56\times10^{9}\exp\left(-\frac{25300}{T_p}\right)\frac{p_{H_2O}}{p_{H_2O}+1.42p_{H2}}C_c \qquad \text{kmol}/\text{m}^3\text{s}$$

- CO_2 gasification (Li and van Heiningen, 1990; Wessel et al., 1997)

$$C + CO_2 = 2CO \qquad \text{Rate} = 6.30\times10^{10}\exp\left(-\frac{30070}{T_p}\right)\frac{p_{CO_2}}{p_{CO_2}+3.4p_{CO}}C_c \qquad \text{kmol}/\text{m}^3\text{s}$$

- Other reactions considered

$$CH_4 + H_2O = CO + 3H_2 \qquad CH_4 + 2O_2 = CO_2 + 2H_2O$$

$$C + 2H_2 = CH_4 \qquad H_2 + \tfrac{1}{2}O_2 = H_2O$$

$$C + \tfrac{1}{2}O_2 = CO \qquad CO + H_2O \leftrightarrow H_2 + CO_2$$

$$CO + \tfrac{1}{2}O_2 = CO_2$$

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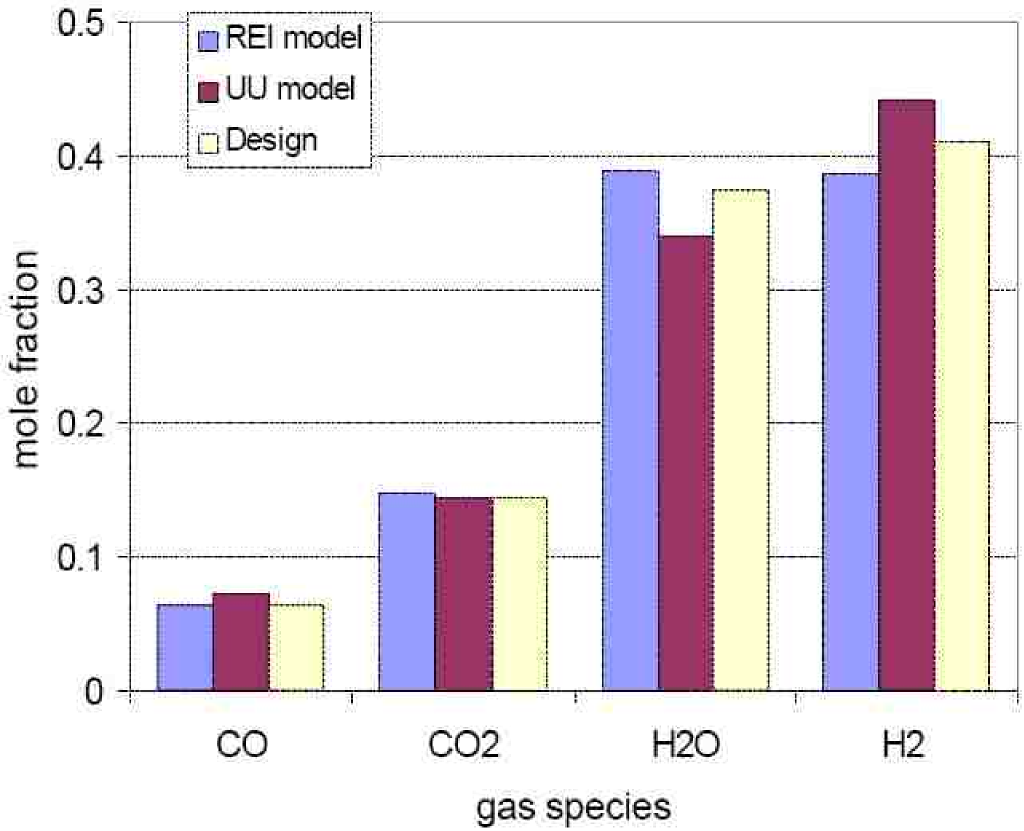
Model Results: Syngas Composition



- ➔ **Model predictions very similar to those of Whitty 2003, based on 10 zones with equal gasification**
- ➔ **Georgia Pacific reports carbon conversion of 95%, while model predicts 99.6%**

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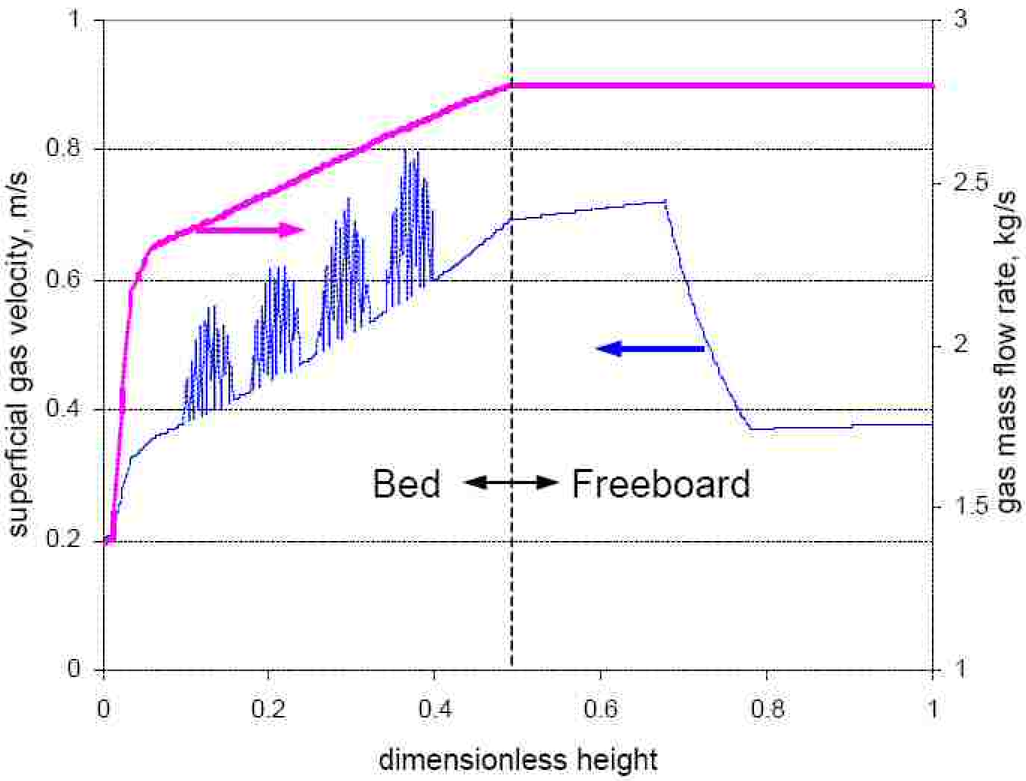
Model Results: Gas Velocity & Mass Flow Rate



- ➔ **Jump increases in both gas mass flow rate and the gas velocity due to moisture vaporization and black liquor pyrolysis**
- ➔ **Spikes in gas velocity inside tube bundles due to changes in cross sectional area of the bed**

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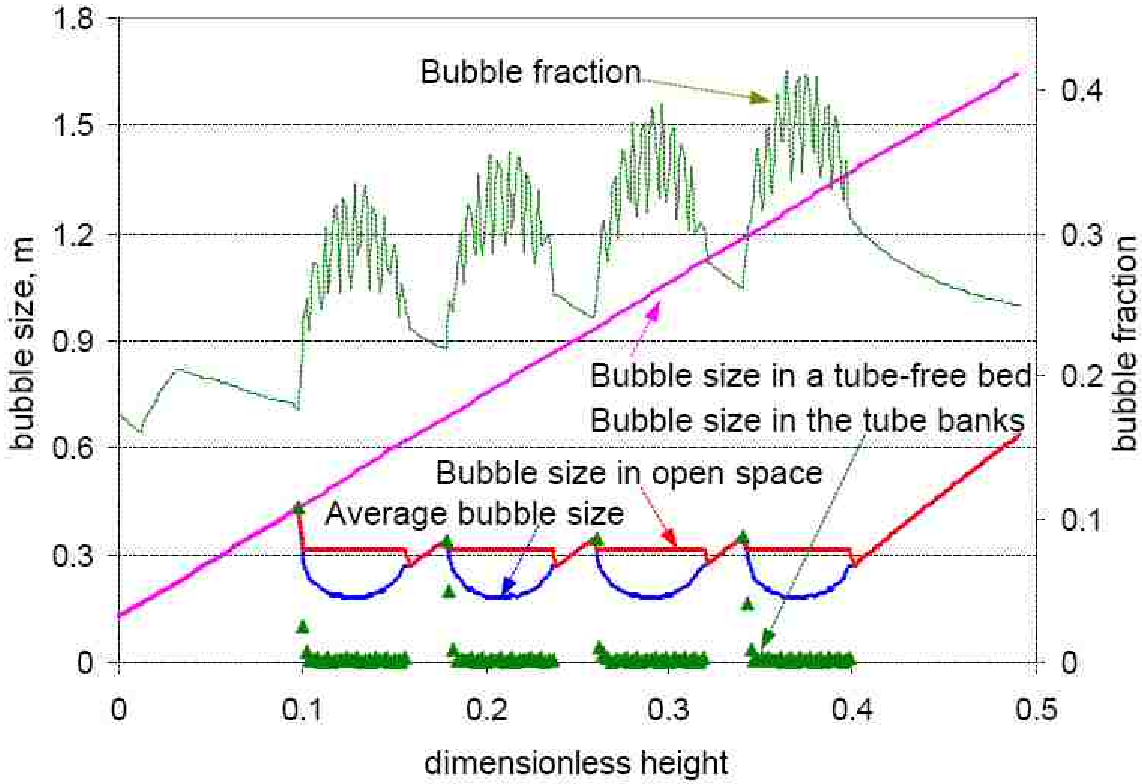
Model Results: Bubble Size and Fraction



Variation of bubble properties with bed height

- Inside the tube bundles, bubble size is similar to the tube pitch
- Bubble fraction ranges from 0.15 to 0.40, where spikes in the tube bank are due to gas velocity increase
- An area-averaged bubble size is used in the model

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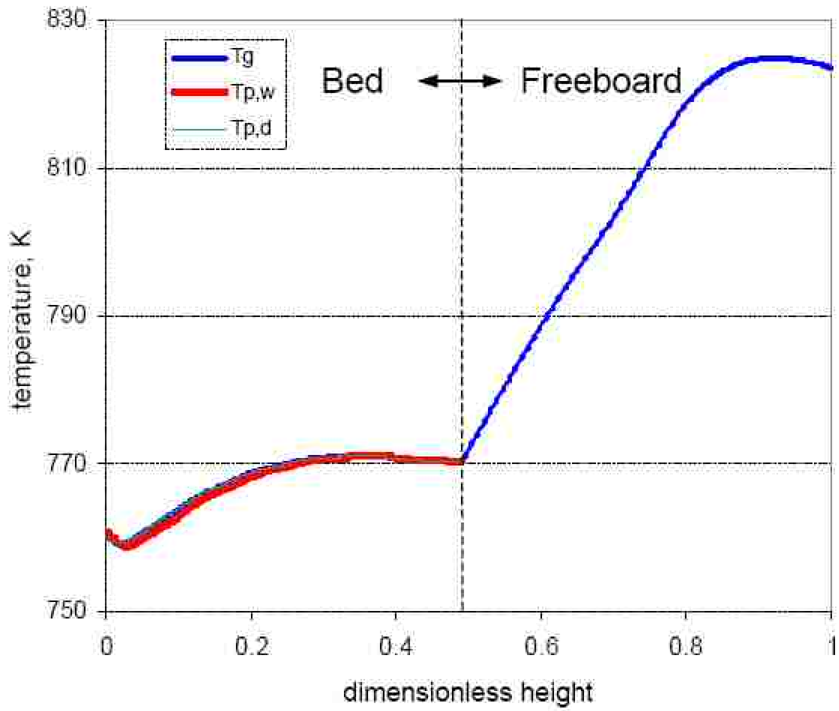
Model Results: Gas and Particle Temperatures



Gas temperature and particle temperature as functions of reactor height

- **Particle temperatures very close to gas temperatures**
- **Vaporization of water near bottom leads to a decrease in temperature, followed by an increase resulting from heat transferred from the pulse combustors**
- **In the freeboard, there are two major reactions:**
  - **exothermic water-gas shift**
  - **endothermic methane-water reforming**

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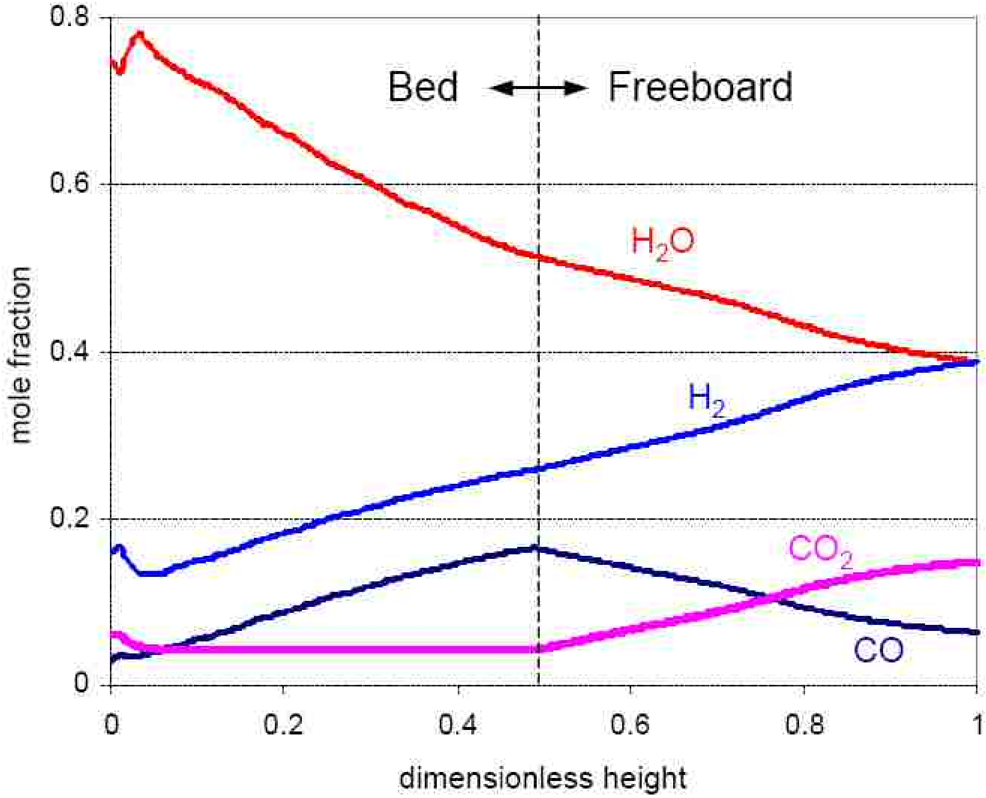
Model Results: Gas Composition



Variation of gas composition with reactor height

- As gasification proceeds, water vapor decreases and CO and hydrogen increases
- In the freeboard, hydrogen and CO2 increase while water vapor and CO decrease
- methane-water reforming is minimal due to low methane concentration

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Model State and Development

- **Currently**
  - The three-phase model provides estimates of syngas concentrations and carbon conversion consistent with the limited data
  - Gas and particle temperature profiles, important for tar formation and bed agglomeration
- **Upcoming**
  - Further validation of the model will be carried out as experimental data become available
  - Effects of operating conditions on the performance of the gasifier will be performed

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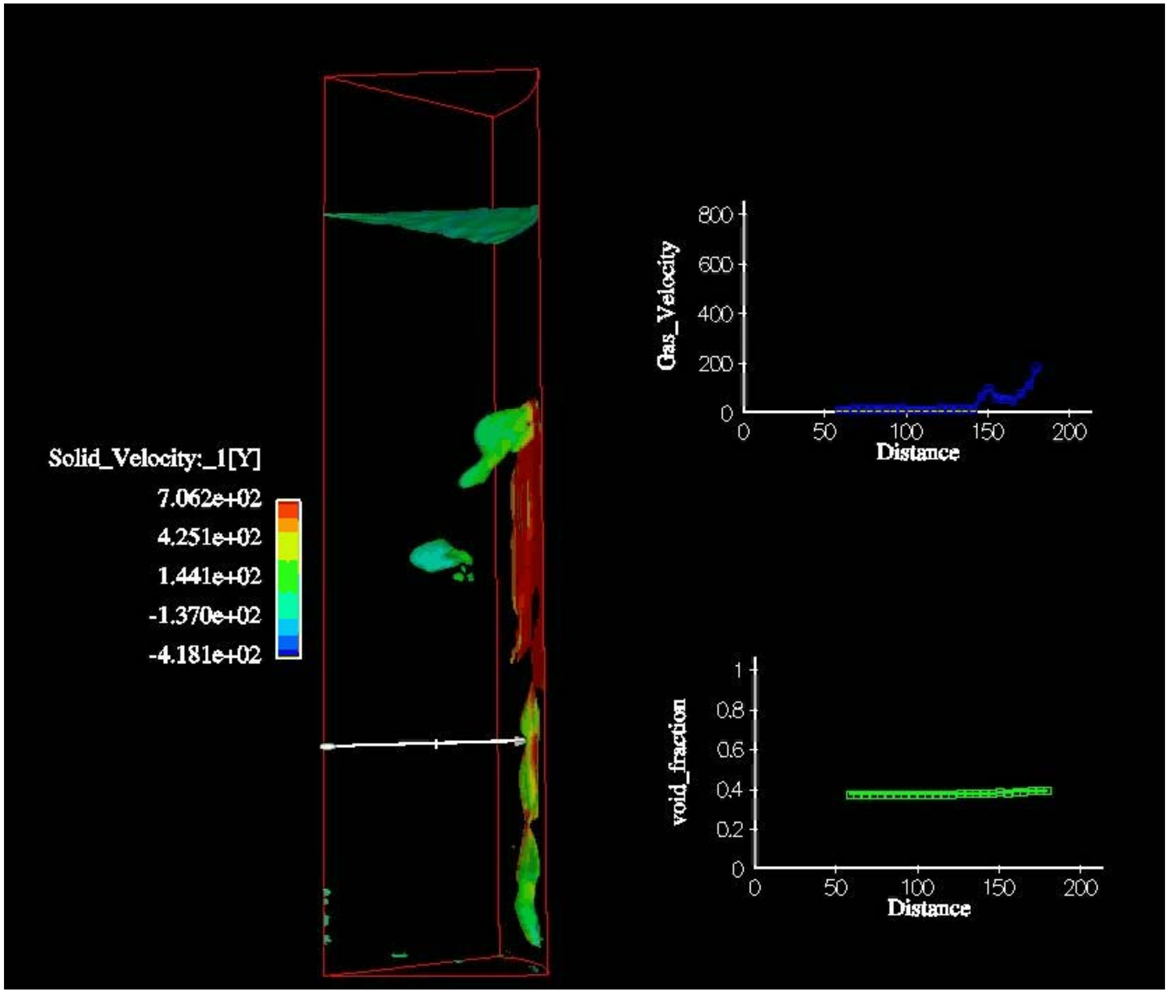
CFD Modeling of FB BLG



- Collaboration with Rand Batchelder
- MFIX code developed at NETL
- Potential for improvements in predictions and evaluation of 3D and transient phenomena

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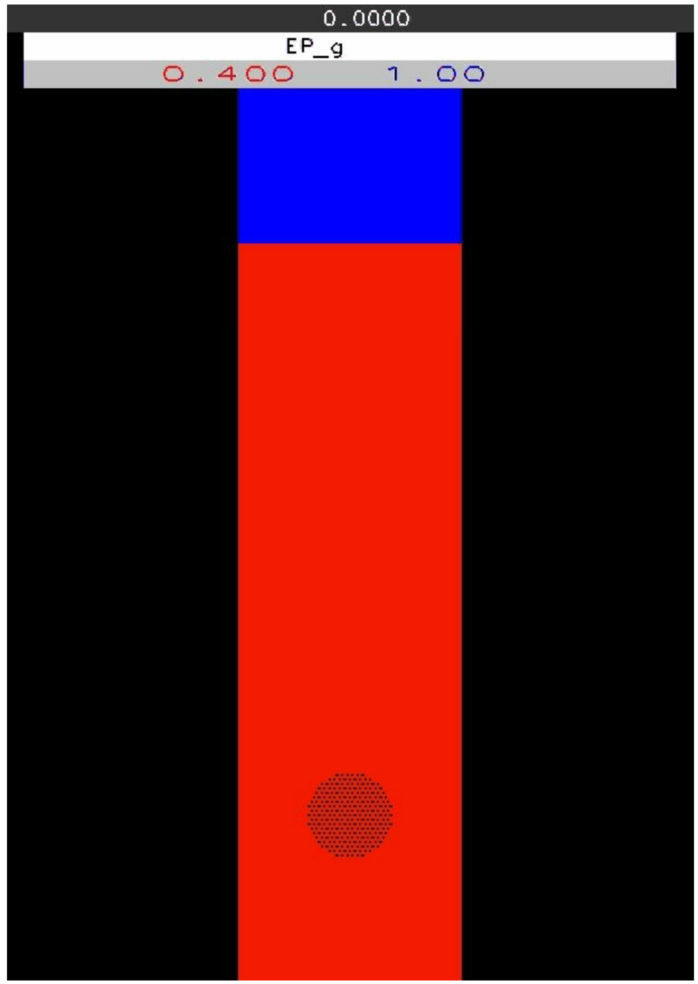
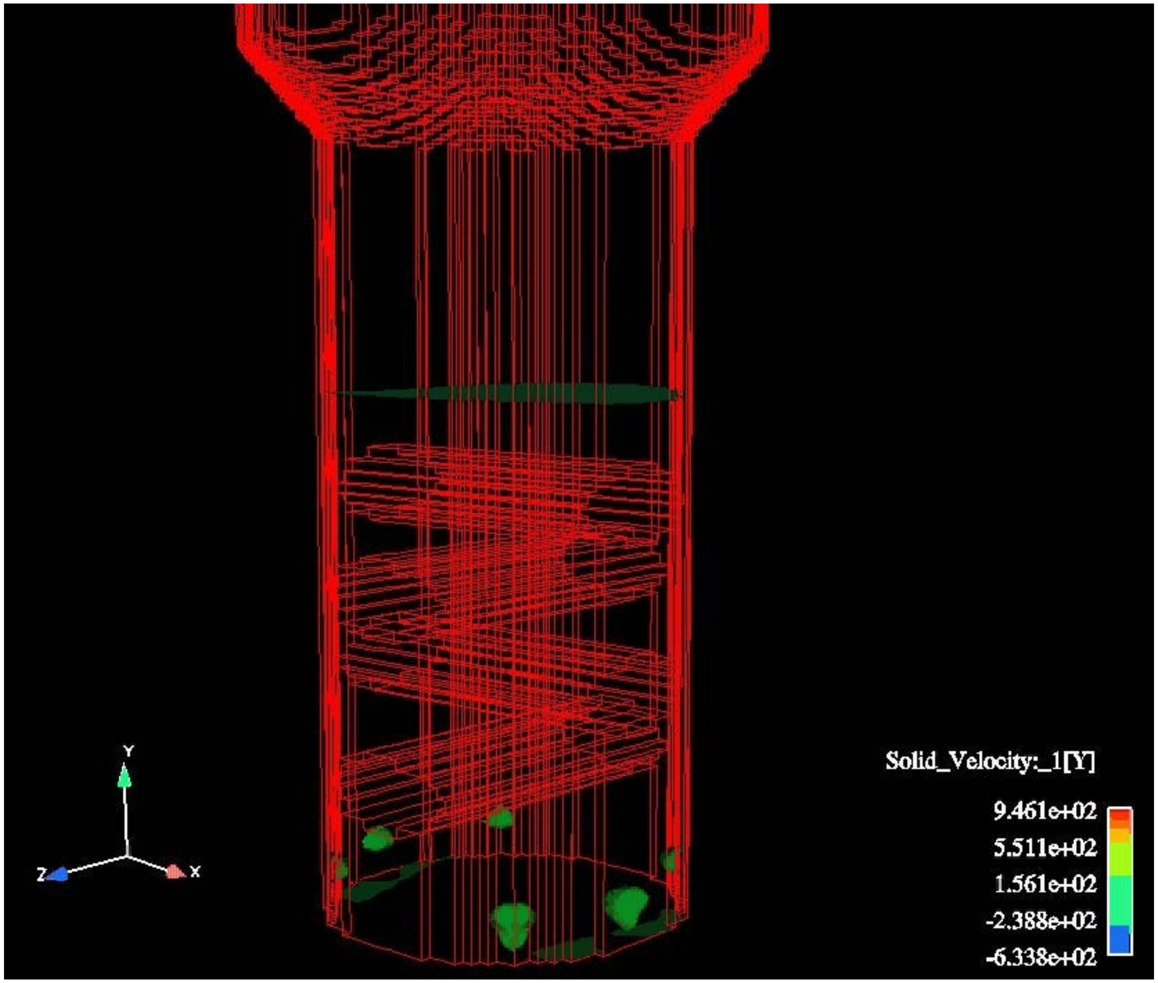
Injector Effects



Tube Bundle Interactions



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