Multiphase Simulation of Entrained Flow Gasification – Modeling Needs

Lanre Oshinowo, Ph.D.
Research & Development/Technology
lanre.oshinowo@conocophillips.com
Oil
Coal
Oil sands
Natural gas
Petroleum coke
Coal bed methane
Transportation fuels
Gas-to-liquids
Gasification
Electricity
Shale oil
LNG

3rd integrated energy company in the U.S
4th largest refiner in the world
6th largest worldwide reserves holder of
National Oil Companies
Outline

• Gas-solids flow in the value chain
• E-Gas™ process overview
• Engineering needs
• Modeling requirements
• Summary
ConocoPhillips Value Chain

Gas Value Chain
- LNG Transport
- LNG Re-gas
- Gas Transport
- Power

Oil Value Chain
- Refining
- Gasification

Value Chain Stages:
- Exploration
- Production
- Transport
- Midstream
- Distribution
- Marketing
- Chemicals
- GTL
- Power
E-Gas™ Gasifier

Raw Syngas

Char Recycle

2nd Stage

First Stage

Slurry

Oxygen

Slurry

Water

Slag

Slag Quench

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Engineering Information Desired

• Inputs
  – Feed – Type, Water content, Solids loading, temperature, Injection…
  – Oxidant – $O_2$ concentration, Temperature

• Outputs
  – Gas flow field – Temperature, velocity, composition
  – Wall conditions – Temperature, heat flux, slag flow
  – Carbon conversion, cold gas efficiency
  – Quantity of carryover – unburned carbon in fly-ash
  – Influence of process, operating conditions and geometric configurations
Coal/Pet coke Gasification

- COAL/PETCOKE
- DEVOLATIZATION
  - Light gases & tar
  - Gas phase reactions
  - $\text{O}_2$
  - $\text{CO/CO}_2$
  - $\text{CO/H}_2$
  - $\text{CO}_2/\text{H}_2\text{O}$
- CHAR COMBUSTION
- CHAR GASIFICATION
- FRAGMENTATION
- SLAG FORMATION

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Multiphase Flow Simulation Needs

- High-fidelity models – detailed geometry and mesh
- Steady-state and transient
- Heat transfer – convective, radiation
- Particle-size distributions, solid collision behavior
- Devolatization kinetics – for range of fuel types
- Detailed kinetic modeling – gas-phase, gas-solid, gas-solid-catalyzed
- Range of flow conditions from high-speed multiphase injection, turbulent combustion, high-viscosity slag flow
- Particle-wall interaction
- Soot production models
- Pollutant models
- Accurate EOS and material properties
Solids Transport

- Relatively high velocity liquid/solid injection
- Particle size distribution of slurry – wetted solids + water
- Fragmentation
- Influence of injector on spray pattern
- Ash deposition and slag transport
- Turbulent dispersion
Devolatization

• Reaction, chemical or network models
• Predictable for any fuel and range of process conditions (T, P)
• Influence on particle transport
  – Solid or porous
Reactions

- Gas-phase
  - Equilibrium
  - Partial equilibrium
  - Full or reduced mechanisms

- Gas-solid
  - Pore-scale modeling
  - Mineral matter
  - Ash formation and inhibition
Turbulence

- Scales
- Transients
- Interaction with solid phase
- Accurate “engineering” models
Speed

- Faster algorithms
- Better parallelization
- Efficient model methods
Value to ConocoPhillips

• A predictive CFD modeling tool could be used to guide engineers to derive much higher improvements in the efficiency and overall cost-savings

• CFD can be used to identify optimal design and reject poorly performing configurations

• Continuously improve the existing technology and design for the future
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Feedback?