CFD Modeling For Entrained Flow Gasifiers

Mike Bockelie, Martin Denison, Zumao Chen, Temi Linjewile, Connie Senior and Adel Sarofim

Reaction Engineering International

Neville Holt
Electric Power Research Institute

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DOE Vision 21 Program
Cost Shared Agreement  DE-FC26-00NT41047
Vision 21 - Computer Simulation

- **Enabling Technology**
- **Benefit**
  - reduce time, cost and technical risk to develop new energyplex systems
    - 100 MW plant ~ 100 – 150 M$
- **Challenges**
  - need for improved component models
    - robust, high fidelity physics based models (CFD)
    - not available for many components for Vision 21 spectrum of conditions
Gasifier Model

- **Model Development**
  - Computational Fluid Dynamic (CFD) + Process models
    - Allows modification of
      - Process conditions, burner characteristics
      - Fuel type, slurry composition
      - gross geometry
    - Generic Configurations:
      - downflow / upflow
      - 1 stage / 2 stage
    - Define Parameters with DOE
      - Improved physical models
        - reaction kinetics
          - high pressure and gasification
        - slag, ash, soot, tar
        - air toxics (metals, PM2.5)

- **Collaboration**
  - N. Holt (EPRI)
  - T.Wall, .... (Black Coal CCSD)
  - K. Hein (IVD)

Vision 21
Modeling Opportunity- Gasifier RAM

• Carbon Conversion & Syngas Quality
  – Fuel Switching
    • Coal, Pet coke, Wastes, Oil, Biomass, Dirt, Blends
  – Fuel Feed System
    • Dry (N2, CO2); Wet (H2O); Pre-heat; Grind size
    • Oxidant: Air vs O2
  – System Modifications / Scale Up
    • Injectors (location, quantity, orientation, spray)
    • Volume (L/D ratio)
    • System pressure

• Slag and Ash Management
  – Viscosity, composition, flux mat’l
  – Carbon content: slag vs flyash

• Refractory Wear
  – Heat extraction

• Transient Operation
  – start-up / shutdown / switching

See Gasification Technologies 2001:
• Stiegel, Clayton and Wimer
• Holt
See Clearwater 2002
• Dogan

Vision 21
Qualifications

- >130 boilers, process furnaces and incinerators in several countries burning a range of fuels including coal, oil, gas, wood, straw, petcoke, tires, hazardous waste

- Complementary relationships with boiler owners, OEMs and service/equipment providers to develop solutions in areas including:
  - NOx Control
  - Corrosion and Deposition
  - Heat flux
  - SOx Control
  - CO, hydrocarbon emissions
  - Carbon-in-flyash
  - Opacity
  - Air toxics (fine particulate, mercury, soot)

- Independent evaluation
## CFD Model

### Inputs
- Geometry
- Wall Properties
- Fuel & Oxidant
  - Properties
  - Composition
    - Ultimate, proximate
    - Ash composition
  - Temperature
  - Particle grind
  - Splits
    - Multiple Injectors
    - Quench

### Outputs = Predicted Values
- Carbon Conversion
- Flow Patterns & Velocities
- Gas & Surface Temperatures
- Gas Species Concentrations
  - Major: CO2, CH4, H2, H2O, N2, O2
  - Minor: H2S, COS, NH3, HCN, ...
  - Reducing vs oxidizing
- Wall Heat Transfer
  - Incident, net flux
  - Backside cooling
- Particle / Droplet Trajectories and Reactions
  - Time temperature histories
  - Wall deposition
  - Flyash (Unburned carbon)
  - Slag
    - Temperature, viscosity, thickness
    - Composition
CFD Model

- **Computer model represents**
  - Gasifier geometry
  - Operating conditions
  - Gasification processes

- **Accuracy depends on**
  - Input accuracy
  - Numerics
  - Representation of physics & chemistry

See Pittsburgh Coal Conference 2002 Paper for model details
Flowing Slag Model

- Model accounts for:
  - Wall refractory properties
  - Back side cooling
  - Fire side flow field + heat transfer
  - Particle deposition on wall
    - Local Deposition Rate
    - Fuel ash properties
    - Composition (ash, carbon)
    - Burning on wall

- Slag model computes
  - $T_{cv}$ = critical viscosity
    - ash composition
  - Slag surface temperature
  - Liquid & frozen slag layer thickness
  - Heat transfer through wall

Based on work by [Benyon], [CCSD], [Senior], [Seggiani]
Flowing Slag Model

Critical Viscosity: Predicted vs Measured

\[ T_{cv} [K] = 3452 - 519.5\alpha + 74.5\alpha^2 - 67.8\beta + 0.86\beta^2 \]

Where \( \alpha = \frac{\text{SiO}_2/\text{Al}_2\text{O}_3}{\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO}} \) and \( \beta = \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO} \)

\( \text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{CaO} + \text{MgO} = 100 \) [weight%]

Measured data from Patterson et al, 2001
### Firing Conditions
- [Benyon, 2002], [Seggiani, 1998]
- Pressure = 25 atm.
- 2600 tpd dried bituminous coal
  - 22% ash
- Dry feed
  - N2:Coal (lb) = 0.075
- Oxidant
  - 76% O2, 11% H2O, 10% N2, 3% Ar
  - O2:C (molar) = 0.46
  - Inlet Stoichiometry ~ 0.4

<table>
<thead>
<tr>
<th>Exit Conditions</th>
<th>Seggiani</th>
<th>Benyon</th>
<th>REI</th>
</tr>
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<tbody>
<tr>
<td>Gas Temp (K)</td>
<td>1803</td>
<td>(1650)</td>
<td>1790</td>
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<tr>
<td>CO (wt %)</td>
<td>76.5</td>
<td>70.9</td>
<td>76.8</td>
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<tr>
<td>CO2 (wt %)</td>
<td>3.2</td>
<td>10.0</td>
<td>6.0</td>
</tr>
<tr>
<td>H2 (wt %)</td>
<td>1.8</td>
<td>1.8</td>
<td>1.9</td>
</tr>
<tr>
<td>H2O (wt %)</td>
<td>-</td>
<td>-</td>
<td>3.2</td>
</tr>
<tr>
<td>N2 (wt %)</td>
<td>-</td>
<td>-</td>
<td>10.1</td>
</tr>
<tr>
<td>Deposition (%)</td>
<td>-</td>
<td>-</td>
<td>4.7</td>
</tr>
<tr>
<td>Carbon Conversion(%)</td>
<td>-</td>
<td>-</td>
<td>~100</td>
</tr>
<tr>
<td>HHV (Btu/lb)</td>
<td>(4431)</td>
<td>(4248)</td>
<td>4622</td>
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<tr>
<td>Cold-Gas Efficiency (%)</td>
<td>-</td>
<td>(91.5)</td>
<td>80.5</td>
</tr>
</tbody>
</table>

(... = estimated value)
Slag Model Summary

Slag Surface Temperature

Liquid Slag Thickness

Solid Slag Thickness

Gas temperature, K

CO

Seggiani

Benyon

REI
Slag Thickness

- curve = camera path
- ball on curve = camera location
- displayed = solid slag thickness
Example: Two Stage – Up Flow

- **Vision 21 Firing Conditions**
  - Pressure = 28 atm.
  - 3000 tpd Illinois #6
    - H2O 11%, Ash 10%
  - Recycle 100 tpd char + ash
  - Slurry: 74% solids (wt.)
  - Slurry Distribution
    - 39%, 39%, 22% (upper)
  - Oxidant
    - 95% O2, 5% N2
    - O2:C (molar) = 0.43
    - Inlet Stoichiometry ~ 0.50

- **Firing System**
  - 4 fuel injectors / level
  - Fuel Injectors ~ pipes

![Diagram of two-stage upflow configuration with labels for upper and lower injectors, jet centerline, and 6D and 0.5D distances.](attachment:diagram.png)
Flow Field

Gas Temperature, K

Axial Velocity, m/s
Gas Composition

H₂  CO  H₂O  CO₂  O₂
Particles and Droplets

Volatile Mass Fraction

Char Mass Fraction

Water Droplet Trajectories
Comparison

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<tr>
<th></th>
<th>Exit</th>
<th>FGR / Cool</th>
<th>NETL</th>
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<td>1335</td>
<td>1311*</td>
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<td>Carbon Conversion, %</td>
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<td>-</td>
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<tr>
<td>Exit LOI, %</td>
<td>0.4</td>
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<td>-</td>
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<td>Deposit LOI, %</td>
<td>28.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Deposition, %</td>
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<td>-</td>
<td>-</td>
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<td>PFR Residence Time, s</td>
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<td>-</td>
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<tr>
<td>Particle Residence Time, s</td>
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<td>-</td>
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<tr>
<td>Water Droplet Res. Time, s</td>
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<td>-</td>
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<tr>
<td>Mole Fraction: CO</td>
<td>43.2%</td>
<td>43.4%</td>
<td>43.5%</td>
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<tr>
<td>H₂</td>
<td>29.2%</td>
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<td>32.5%</td>
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<td>H₂O</td>
<td>16.7%</td>
<td>16.7%</td>
<td>13.6%</td>
</tr>
<tr>
<td>CO₂</td>
<td>8.3%</td>
<td>8.5%</td>
<td>8.6%</td>
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<tr>
<td>H₂S</td>
<td>0.8%</td>
<td>-</td>
<td>-</td>
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<tr>
<td>COS</td>
<td>0.0%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N₂</td>
<td>1.7%</td>
<td>1.7%</td>
<td>0.9%</td>
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<td>Exit Mass Flow, klb/hr</td>
<td>483</td>
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<td>HHV of Syngas, Btu/lb</td>
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<tr>
<td>HHV of Syngas, Btu/SCF</td>
<td>237</td>
<td>-</td>
<td>250*</td>
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<tr>
<td>Cold-Gas Efficiency</td>
<td>78.0%</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

V21 “Design” Conditions

- DOE-NETL flow sheet analysis of “DESTEC-style” 2 stage gasifier in an IGCC plant
- Syngas:
  - At Gasifier exit (*):
  - Gas Composition after GCU:

Minor Species:

\[ \text{NH}_3, \text{HCN}, \text{O}, \text{OH}, \text{CH}, \text{CH}_4, \text{C}_2\text{H}_2, \text{H}, \text{N}, \text{HCl}, \text{H}_2\text{S}, \text{COS} < 1 \% \]
Single Stage – Down Flow

- **Vision 21 Firing Conditions**
  - Pressure = 32 atm.
  - 3000 tpd Illinois #6
    - H2O 11%, Ash 10%
  - Slurry: 74% solids (wt.)
  - Oxidant
    - 95% O2, 5% N2
    - O2:C (molar) = 0.46
    - Inlet Stoichiometry ~ 0.51
Gas, Particle and Droplet Flows

- Gas Temp., K
- Axial Gas Velocity, m/s
- Particle Coal Fraction
- Particle Char Fraction
- Water mole fraction
- $\text{H}_2$
Compare

<table>
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<tr>
<th></th>
<th>Exit</th>
<th>cool/clean</th>
<th>NETL</th>
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<tbody>
<tr>
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<td>1641</td>
<td>-</td>
<td>1650*</td>
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<td>Carbon Conversion, %</td>
<td>98.3</td>
<td>-</td>
<td>-</td>
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<td>Exit LOI, %</td>
<td>6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Deposit LOI, %</td>
<td>33</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Deposition, %</td>
<td>3</td>
<td>-</td>
<td>-</td>
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<tr>
<td>PFR Residence Time, s</td>
<td>1.41</td>
<td>-</td>
<td>-</td>
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<tr>
<td>Particle Residence Time, s</td>
<td>0.20</td>
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<td>-</td>
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<td>Water Droplet Res. Time, s</td>
<td>0.01</td>
<td>-</td>
<td>-</td>
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<td>Mole Fraction: CO</td>
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<td>41.3%</td>
<td>41.8%</td>
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<td>28.2%</td>
<td>30.8%</td>
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<td></td>
<td>17.3%</td>
<td>15.1%</td>
<td>15.3%</td>
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<td>8.6%</td>
<td>10.1%</td>
<td>10.2%</td>
</tr>
<tr>
<td></td>
<td>0.8%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>0.0%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>1.7%</td>
<td>1.7%</td>
<td>0.9%</td>
</tr>
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<td>Exit Mass Flow, klb/hr</td>
<td>525</td>
<td>-</td>
<td>524*</td>
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<td>HHV of Syngas, Btu/lb</td>
<td>4508</td>
<td>-</td>
<td>-</td>
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<tr>
<td>HHV of Syngas, Btu/SCF</td>
<td>236</td>
<td>-</td>
<td>240*</td>
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<tr>
<td>Cold-Gas Efficiency</td>
<td>78.8%</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

- **V21 “Design” Conditions**
  - DOE flow sheet analysis of “Texaco-style” 1 stage gasifier in an IGCC plant
  - **Syngas**:
    - At Gasifier exit (*):
    - Gas Composition after GCU:
      - \( T = 843 \text{ K} \) (1060F)

**Minor Species**:

\[ \text{NH}_3, \text{HCN}, \text{O}, \text{OH}, \text{CH}, \text{CH}_4, \]
\[ \text{C}_2\text{H}_2, \text{H}, \text{N}, \text{HCl}, \text{H}_2\text{S}, \text{COS} < 1 \% \]
## Fuel Switch – Petcoke

### New Firing Conditions
- Match syngas BTU/hr from Illinois #6 case
- Flow rates:

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Illinois#6</th>
<th>Petcoke</th>
<th>%Change</th>
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</thead>
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<tr>
<td>Fuel (tpd)</td>
<td>3089</td>
<td>2569</td>
<td>-16.8%</td>
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<tr>
<td>Oxidant (tpd)</td>
<td>2535</td>
<td>1965</td>
<td>-22.5%</td>
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<tr>
<td>(O_2):C Mole Ratio</td>
<td>0.459</td>
<td>0.365</td>
<td>-20.5%</td>
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<tr>
<td>(H_2O):C Mole Ratio</td>
<td>0.465</td>
<td>0.499</td>
<td>7.3%</td>
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<table>
<thead>
<tr>
<th>Outputs</th>
<th>Illinois#6</th>
<th>Petcoke</th>
<th>%Change</th>
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<td>Exit Temperature, K</td>
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<td>Carbon Conversion, %</td>
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<td>6</td>
<td>11</td>
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<td>40</td>
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<td>Deposition, %</td>
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<td>2</td>
<td></td>
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<td>(H_2)</td>
<td>28.2%</td>
<td>28.5%</td>
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<td>(H_2O)</td>
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<td>(CO_2)</td>
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<td>(H_2S)</td>
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<td>1.2%</td>
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<tr>
<td>COS</td>
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<td>(N_2)</td>
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<td>1.5%</td>
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<td>Cold-Gas Efficiency</td>
<td>78.8%</td>
<td>83.4%</td>
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</table>
Gasifier Process Model

- Fast running Process Model for Gasifier
  - Design inputs for CFD model
  - Indicator for proper slag flow

- Consists of two submodels
  - Zonal Equilibrium model
  - Particle burnout model

- Iterate between the submodels
Summary

- CFD models for entrained flow gasifiers
  - Mechanistic based approach
  - Analysis tool to address broad range of operational and design problems for gasifiers
- Comparisons to available information
  …getting better …
- Next?
  - Improve
    - slag (mineral matter, heat extraction), soot, air toxics
    - gasification kinetics
  - Applications
    - Operations: fuel switching (Petcoke, blends)
    - R+D questions: feed type, volume,…
  - Impact of syngas on downstream equipment & process
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REI

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Zumao Chen, Temi Linjewile, Connie Senior, Adel Sarofim, REI Technical Staff
- Develop component models, workbench, …. 

Collaborators

Neville Holt (EPRI)
Gasifier System Configurations & Validation

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Coal Gasification Data and Mineral Matter Sub-models

Klaus Hein, Bene Risio (U. Stuttgart/IVD, RECOM)
transient gasifier simulations, gasification in the EU
Questions, Comments, Suggestions.....

bockelie@reaction-eng.com