Modeling of Industrial Fluidized Systems using Barracuda Virtual Reactor®

Albuquerque, New Mexico

Monday (8:30 AM – 5:00 PM)
- Introduction to Barracuda VR
- Kuipers Bed Training Problem Setup
- Kuipers Bed Training Problem Post Processing

Tuesday (8:30 AM – 4:30 PM)
- Tuesday Gasifier Introduction
- Tuesday Gasifier Gridding
- Tuesday Gasifier Project Setup
- Chemistry Introduction
- Chemistry Volume Average Setup
- Chemistry Discrete Particle Introduction
- Chemistry Discrete Particle Setup

Wednesday (8:30 AM – 4:30 PM)
- Tuesday Gasifier Post Processing
- Wednesday Gasifier Project Setup

Thursday (8:30 AM – 4:30 PM)
- Wednesday Gasifier Advanced Post Processing
- Optional training presentations or customer project time:
  - Cyclone
  - CFB Erosion
  - 2D Gasification

Friday (8:30 AM – 12:00 PM)
- Best Practices
- Customer Project Wrap-Up

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Customer Feedback Form

New User Training Class

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Thank you for participating in the **Barracuda VR™** New User Training Class. We appreciate any feedback regarding the content and presentation. Thank you for taking the time to respond to the questions below. Your comments are very helpful to us. Please mail or fax your response to us.

1. Please rate the <u>overall</u> quality of the training seminar by circling the appropriate response:

   Very poor   Below Expectations   Above Expectations   Outstanding

   Comments:

2. Please rate the quality of the training <u>material</u> by circling the appropriate response:

   Very poor   Below Expectations   Above Expectations   Outstanding

   Comments:

3. Please rate the quality of the <u>presentation</u> by circling the appropriate response:

   Very poor   Below Expectations   Above Expectations   Outstanding

   Comments:

Continued on next page

4. Was the information presented in a clear, structured and useful manner?

Yes No

Comments:

5. How would you rate the pace of presentation?

Too Much / Too Fast Just Right Too Little / Too Slow

Comments:

6. Do you feel that you can now independently setup a **Barracuda** project, run simulations, and understand the graphical results?

Yes No With some User Support

Comments:

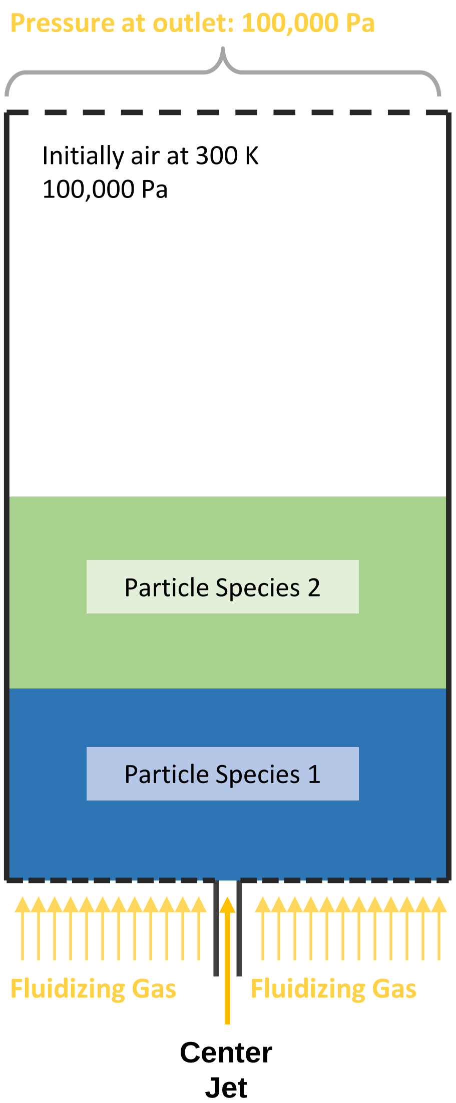
7. Have your expectations been met?

Not Met Met Exceeded

Comments:

8. Additional Comments and/or Suggestions for Future Application Areas:

Kuipers Bed Process Sheet

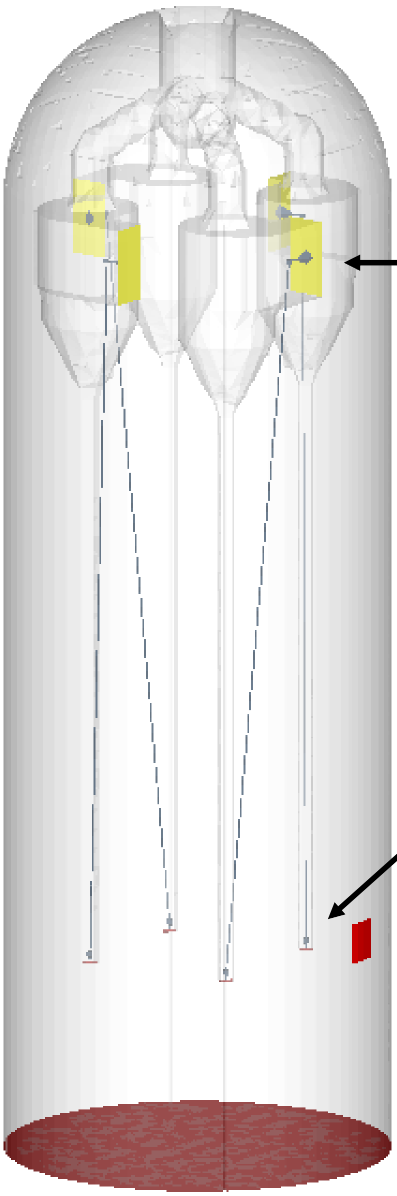


- Geometry
  - 57 cm wide
  - 1.5 cm deep
  - 100 cm total height
  - 50 cm initial bed height
  - 1.5 cm X 1.5 cm jet centered at bottom
- Temperature
  - Isothermal at 300 K
- Particles
  - Use two identical particle species to view mixing behavior
  - Material density 2.66 g/cm3 (glass beads)
  - Diameter: 440µm - 560µm. This is 500 µm ±12%
- Initial conditions
  - Fluid phase: air at rest at atmospheric pressure
  - Solid phase: particles in bottom ½ of bed at close-pack (θcp = 0.55)
- Boundary conditions
  - Fluid
    - Grid velocity: 0.25 m/s
    - Center jet velocity: 10 m/s
    - Top open to atmosphere
  - Particles
    - Cannot enter or leave

Tuesday Gasifier Process Sheet

- Isothermal at 1300 K
- No chemistry in this model

Boundary	Fluid Flow	Particle Flow
Fluidizing Air + Steam	Velocity = 0.3 m/s Gas (mass fractions): $0.3\ H_2O$, $0.54\ N_2$, $0.16\ O_2$	None
Fresh Coal Feed	Velocity = 0.25 m/s Gas (mass fractions): $0.77\ N_2$, $0.23\ O_2$	Fresh coal at 1 kg/s
Cyclone Diplegs	Controlled by BC Connector	Controlled by BC Connector



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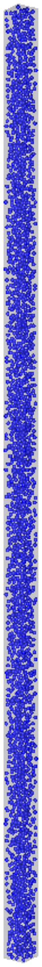
Volume Average Chemistry Process Sheet

- 1 cm x 1cm x 40 cm dimensions
- Tube filled with 200 µm diameter coal particles
- Coal particle locations are fixed in space with a volume fraction of 0.4 and initial temperature of 975 K
- Coal is assumed to be 90% carbon and 10% ash (SiO2)
- Pure steam enters bottom of tube at 1 cm/s and 800 K. Use volume average chemistry for this model.



Forward Reaction

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2}$$

$$\frac{d[\mathrm{CO}]}{dt} = \left(219\ \frac{\mathrm{m}^3}{\mathrm{kg\,K\,s}}\right) T \exp\left(\frac{-22645\mathrm{K}}{T}\right) \rho_{\mathrm{C}}\, [\mathrm{H_2O}]$$

Reverse Reaction

$$\mathrm{CO} + \mathrm{H_2} \longrightarrow \mathrm{C} + \mathrm{H_2O}$$

$$\frac{d[\mathrm{H_2O}]}{dt} = \left(15.7\ \frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2 \exp\left(\frac{-33190\ \mathrm{K}}{T}\right) \rho_{\mathrm{C}}\, [\mathrm{H_2}]\, [\mathrm{CO}]$$

Note: If gas concentration units are **mol/m³**, the reaction rate units will become **mol/m³/s**

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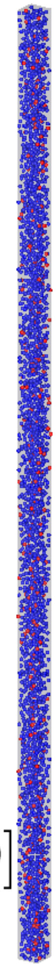
Discrete Chemistry Process Sheet



- 1 cm x 1cm x 40 cm dimensions
- Tube filled with 200 µm diameter coal particles
- Coal particle locations are fixed in space with a volume fraction of 0.4 and initial temperature of 975 K
- Coal is assumed to be 90% carbon and 10% ash (SiO2)
- Steam containing 10% by volume fine coal particles (20 µm) enters the bottom of tube at 1 cm/s and 800 K. Fine coal particles pass through the interstitial spaces in the fixed coal bed. Use discrete particle chemistry for this model.

Forward Reaction

$$\mathrm{C} + \mathrm{H_2O} \longrightarrow \mathrm{CO} + \mathrm{H_2}$$

$$\frac{d\,[\mathrm{C}(s)]}{dt} = -\underbrace{\left(219\,\frac{\mathrm{m}^3}{\mathrm{kg\,K\,s}}\right) T\theta_f \exp\left(\frac{-22645\mathrm{K}}{T}\right) m_{\mathrm{C}}}_{\text{Rate Coefficient}}\,[\mathrm{H_2O}]$$

Reverse Reaction

$$\mathrm{CO} + \mathrm{H_2} \longrightarrow \mathrm{C} + \mathrm{H_2O}$$

$$\frac{d\,[\mathrm{C}(s)]}{dt} = \underbrace{\left(15.7\,\frac{\mathrm{m}^6}{\mathrm{kg\,mol\,K^2\,s}}\right) T^2\theta_f \exp\left(\frac{-33190\,\mathrm{K}}{T}\right) m_{\mathrm{C}}}_{\text{Rate Coefficient}}\,[\mathrm{H_2}]\,[\mathrm{CO}]$$

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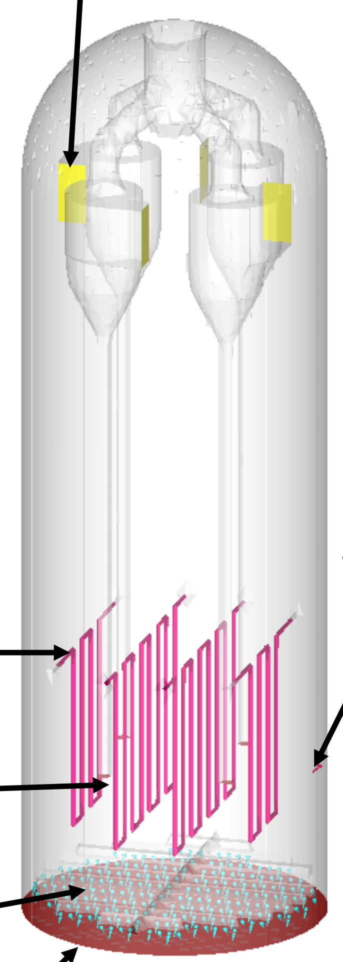
Wednesday Gasifier Process Sheet

- Thermal calculations are enabled, initial temperatures of particles and gas in bed set to 1300 K
- Chemical reactions are included
- Initial bed mass is 4800 kg
- Initially filled with N_2 at 200 kPa

Boundary	Fluid Flow	Particle Flow
Fluidizing Air	Mass flow rate = 0.691 kg/s Temperature = 700 K Gas (mass fractions): 0.77 N_2, 0.23 O_2	None
Steam Sparger through 204 injection nozzles	Mass flow rate = 0.296 kg/s Velocity = 10 m/s Temperature = 900 K Gas: pure H_2O	None
Fresh Coal Feed	Mass flow rate = 5 g/s Velocity = 5 m/s Temperature = 500 K Gas (mass fractions): 0.77 N_2, 0.23 O_2	Fresh coal at 1 kg/s
Cyclone Diplegs	Velocity = 0.5 m/s Temperature = 1300 K Gas: pure N_2	Cyclone dipleg particles with flow rate set to match elutriation into each cyclone.



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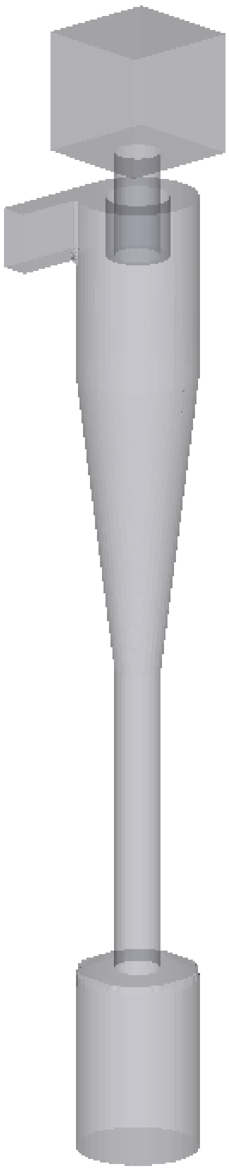
Chemical Reactions

Reaction	Stoichiometric Equation	Reaction Rate Expression (mol m^{-3} s^{-1})	Source
Steam gasification	$C(s)+H_2O \rightarrow CO+H_2$	$r_{1,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[H_2O]$	Syamlal, 1992
	$CO+H_2 \rightarrow C(s)+H_2O$	$r_{1,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-6{,}319}{T}-17.29\right)[H_2][CO]$	
CO_2 gasification	$C(s)+CO_2 \rightarrow 2CO$	$r_{2,f} = 6.36 m_C T \exp\left(\frac{-22{,}645}{T}\right)[CO_2]$	Syamlal, 1992
	$2CO \rightarrow C(s)+CO_2$	$r_{2,r} = 5.218\times10^{-4} m_C T^2 \exp\left(\frac{-2{,}363}{T}-20.92\right)[CO]^2$	
Methanation	$0.5C(s)+H_2 \rightarrow 0.5CH_4$	$r_{3,f} = 6.838\times10^{-3} m_C T \exp\left(\frac{-8{,}078}{T}-7.087\right)[H_2]$	Syamlal, 1992
	$0.5CH_4 \rightarrow 0.5C(s)+H_2$	$r_{3,r} = 0.755 m_C T^{0.5} \exp\left(\frac{-13{,}578}{T}-0.372\right)[CH_4]^{0.5}$	
Combustion	$2C(s)+O_2 \rightarrow 2CO$	$r_4 = 4.34\times10^7 \theta_C T \exp\left(\frac{-13{,}590}{T}\right)[O_2]$	Yoon, 1978
Water gas- shift	$CO+H_2O \rightarrow CO_2+H_2$	$r_{5,f} = 7.68\times10^{10} \exp\left(\frac{-36{,}640}{T}\right)[CO]^{0.5}[H_2O]$	Bustamante, 2005
	$CO_2+H_2 \rightarrow CO+H_2O$	$r_{5,r} = 6.4\times10^9 \exp\left(\frac{-39{,}260}{T}\right)[H_2]^{0.5}[CO_2]$	Bustamante, 2004

Cyclone Process Sheet



- Geometry
  - 0.2 m maximum diameter
- Temperature
  - Isothermal at 300 K
- Particles
  - Chalk powder, particle density = 2730 kg/m3
  - Bulk density = 0.5 particle density
  - PSD provided
  - Loading = 50 g/m3 of air
- Fluid
  - Air
  - Gas flow = 0.04 m3/s
- Boundary Conditions
  - Flow BC - Solids can enter at inlet
  - Pressure BC - solids exhaust at the vortex tube only

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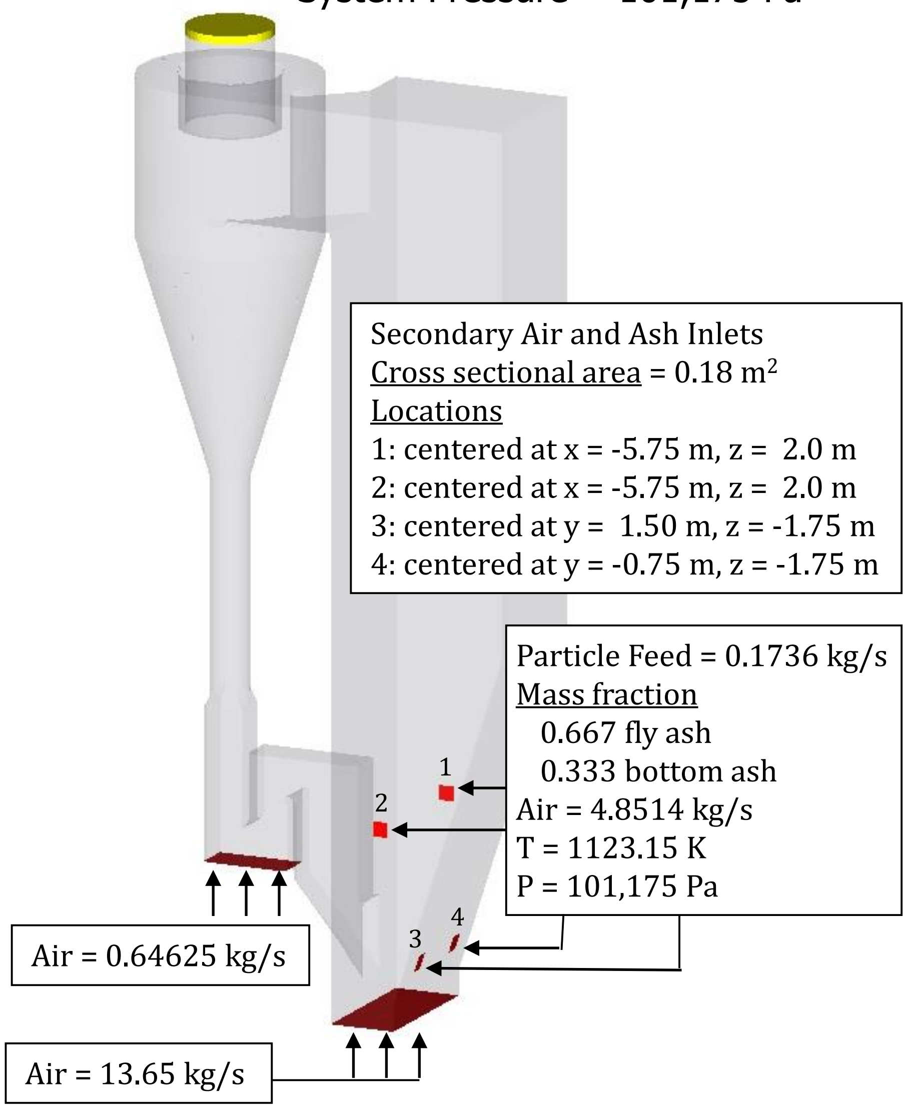
CFB Erosion Process Sheet

System Pressure = 101,175 Pa



- Materials Required
  - Air, SiO_2, and Ash
- Particle Species
  - Sand (SiO_2): $\rho = 2650$ kg/m^3 and dp = 60 – 480 µm
  - Fly ash: $\rho = 1500$ kg/m^3 and dp = 10 – 480 µm
  - Bottom ash: $\rho = 1500$ kg/m^3 and dp = 18 – 2200 µm
  - Full PSD for each provided
  - Close pack volume fraction, $\Theta_{cp} = 0.55$
- Model Assumptions
  - Isothermal flow at 1123.15 K
  - A simulation run time of 40 seconds should be sufficient to study erosion
  - Particles can exit through the cyclone outlet

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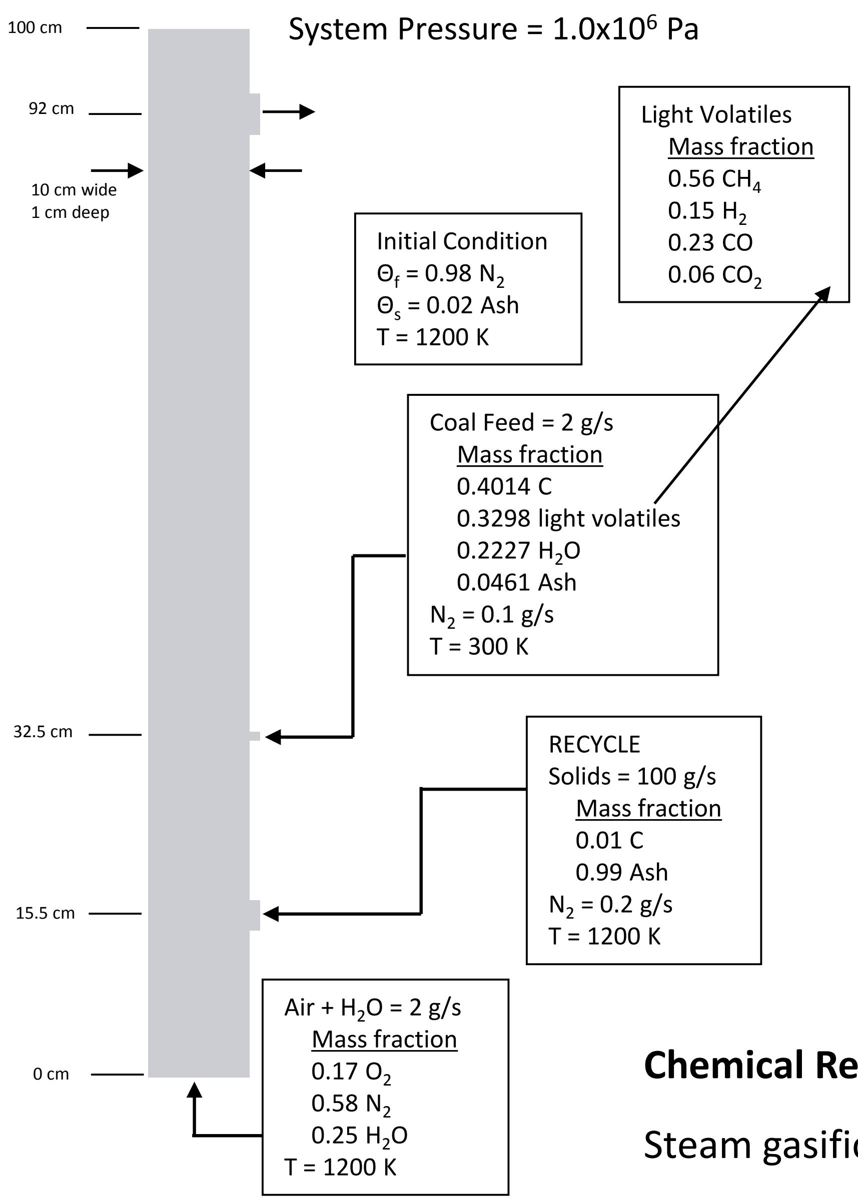
2D Gasifier Process Sheet



Chemical Reactions for Gasifier

Steam gasification: $C + H_2O \leftrightarrow CO + H_2$

CO2 gasification: $C + CO_2 \leftrightarrow 2\ CO$

Methanation: $0.5\ C + H_2 \leftrightarrow 0.5\ CH_4$

Carbon combustion: $2\ C + O_2 \rightarrow 2\ CO$

Water gas-shift: $CO + H_2O \leftrightarrow CO_2 + H_2$

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