Thermal Reacting Gasifier
Part 1: Presentation

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Training Objectives

This training exercise adds more realism and complexity to the gasifier model defined yesterday.

- More internal geometries are included: gas sparger and heating coils
- Injection points are added to introduce fresh coal and steam into the system
- Chemistry and thermal calculations are added

Set up a complex model based on a previously defined simplified model.

- Copy a project file to a new location using Save Case As…
- Modify the grid as necessary
- Add chemistry and thermal definitions to project

Use several newly introduced features of Barracuda.

- Thermal calculations
- Injection BCs
- Chemical reactions

What do we want to learn from this model?

Always keep in mind why you are running any model.

For the previous, simplified gasifier training problem, we wanted to learn the following:

- General fluidization characteristics
- Entrainment rate of particles

For this more complex model, we would like to additionally study:

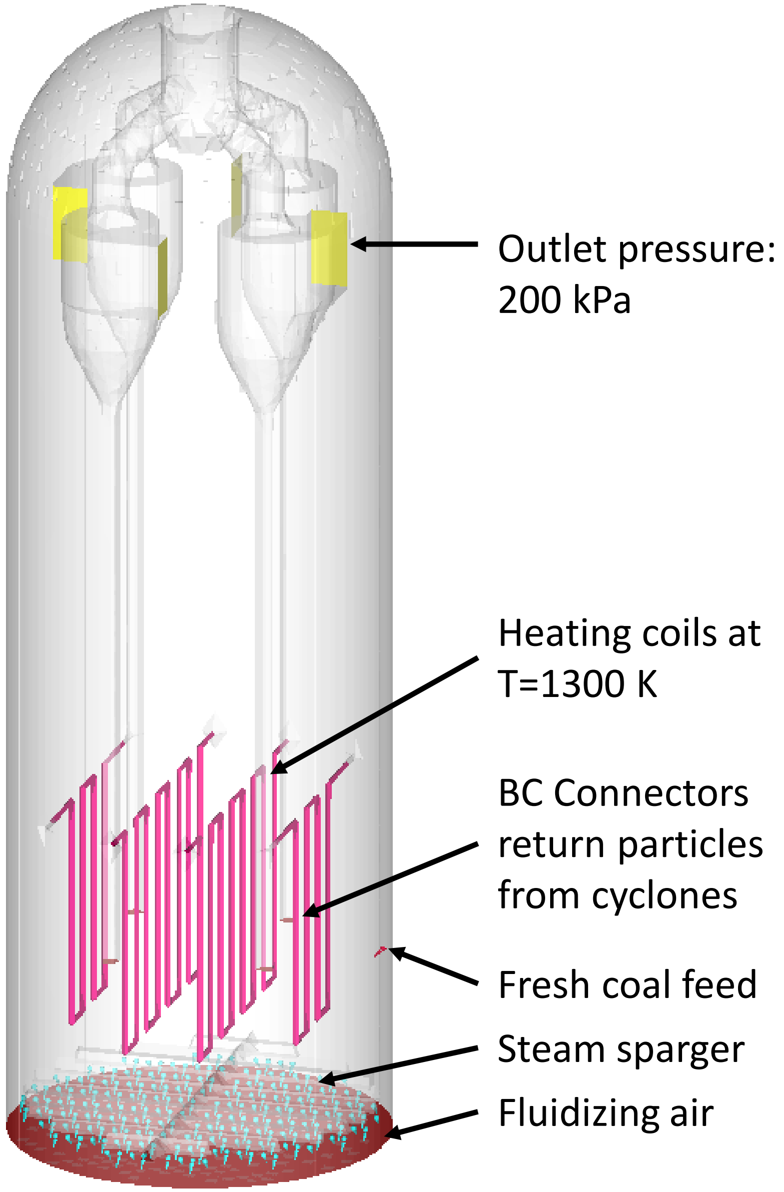
- Are there any hot-spots in the bed?
- What is the gas composition leaving the cyclones?
- Did the addition of thermal and chemistry affect the conclusions drawn based on studying results of the simplified model?

Process Sheet

Thermal calculations are enabled, initial temperature of particles and gas in bed set to 1300 K.

Chemical reactions are included.

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 = 5e-3 kg/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	Controlled by BC Connector	Controlled by BC Connector

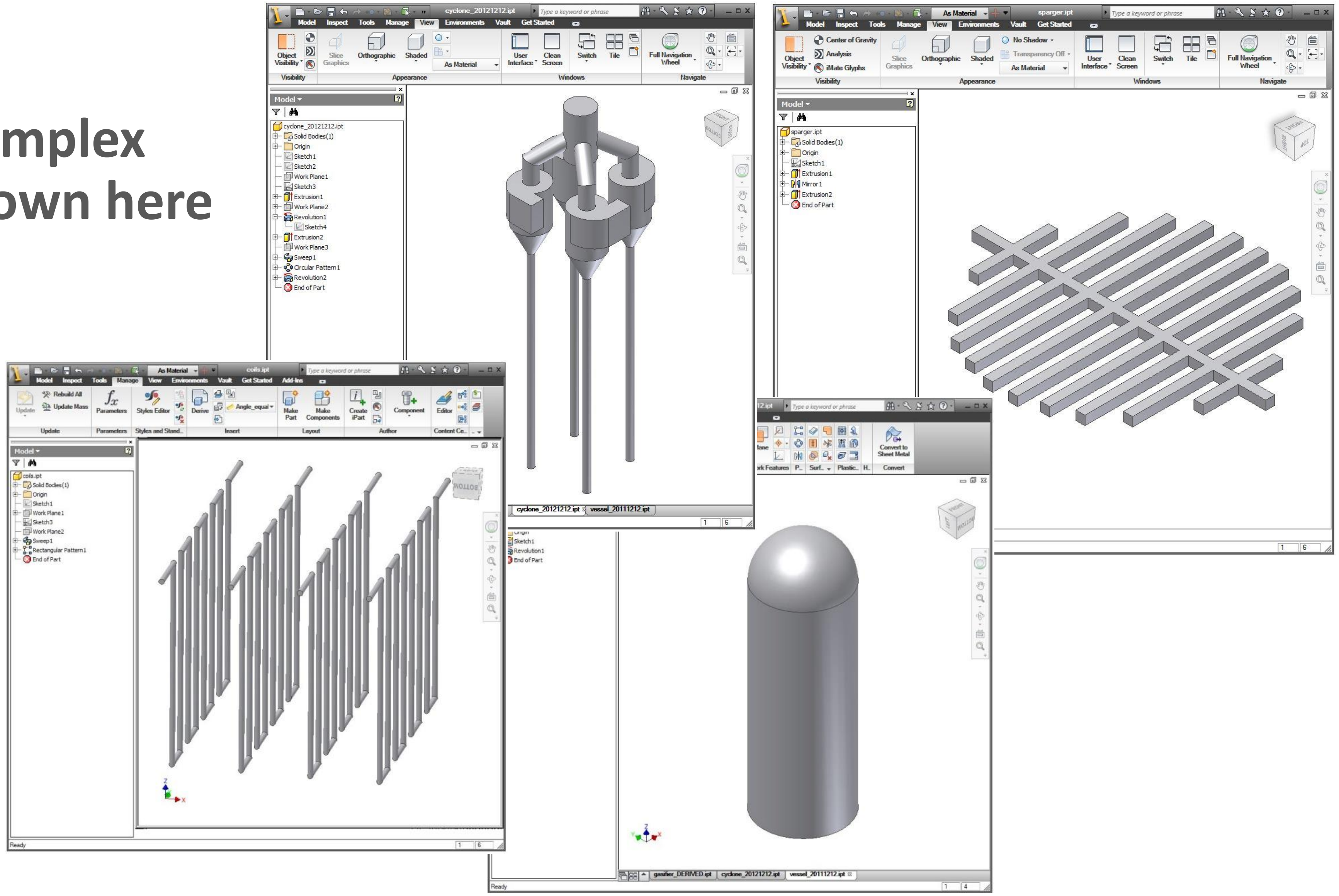


Chemical Reactions

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

More Complex Geometry

To create the CAD for this complex geometry, the solid parts shown here were created.



Final STL File with Internal Structures Subtracted

The cyclones, gas sparger, and heating coils were subtracted from the vessel.

The example here was made with Autodesk Inventor, using a Derived Part based on an assembly of the individual parts.

This resulted in a solid model of the internal flow volume in which particles and fluid can travel.

Remember: we need a model of the interior flow volume. We do not want a "thin-walled" geometry.