Gasifier Training Problem Part 1: Introduction

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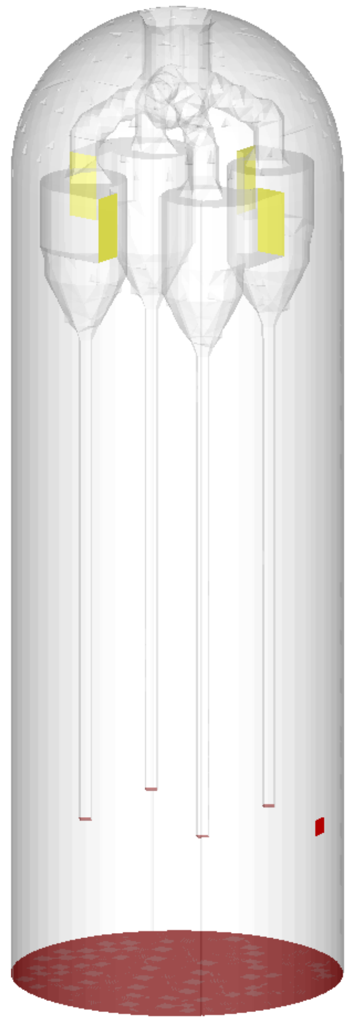
Training Objectives

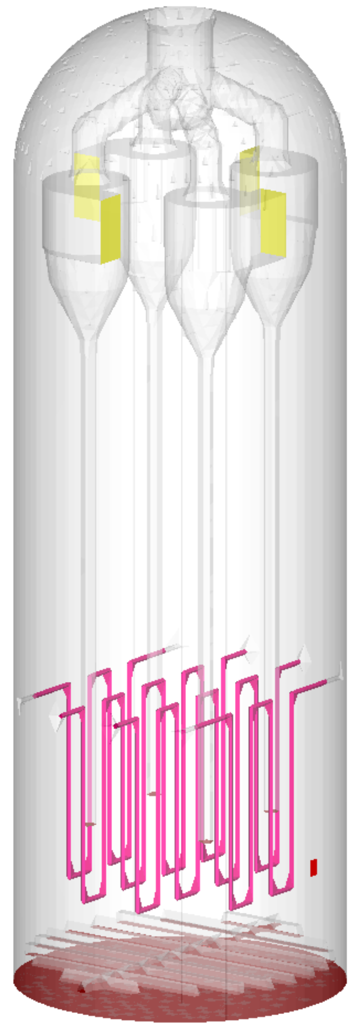
- Introduction to complex Barracuda model (coal gasifier)
- General modeling & simulation principles
    - Why are we running a simulation?
    - What do we want to learn?
    - What level of detail is required?
    - What amount of time needs to be simulated?
    - What simplifications can be made?
- Strategies for getting useful answers quickly
    - Detailed models vs “workhorse models”
    - Run coarse models before detailed models

Barracuda Training Coal Gasifier

- The purpose of this model is to provide a realistic example of the types of systems that people typically model using Barracuda.
- Complex geometry
    - Internal cyclones
    - Internal heating coils
    - Internal gas sparger
- Complex operating conditions
    - Multiple gas inlets and outlets
    - Multiple particle inlets and outlets
    - Chemistry and thermal are important
- For training, we will define 2 models:
    - Coarse, isothermal, non-reacting case that runs fast
    - More detailed, chemistry + thermal case



Simplified geometry, isothermal



Complex geometry, thermal + chemistry

Questions to Ask About Every Simulation You Run

- Why are we running a simulation?
  - Designing a new process and want to predict performance through simulations.
  - Trouble-shooting a problem with an existing process and want to understand the cause of the problem better.
- What do we want to learn from the simulation?
  - Answers to this question will determine much of the data output you need to select during your Barracuda project setup.
  - Solids entrainment? -> Make sure you define flux planes.
  - Erosion on walls? -> Make sure you turn on the wall erosion model.
  - Temperature profile? -> Make sure to select thermal output variables.

Questions to Ask About Every Simulation You Run

- What level of detail is required?
  - Depending on what your goals are for a simulation, more or less detail may be required.
  - Overall fluidization behavior might be captured well by a fairly coarse, fast-running model.
  - Detailed flow behavior around small geometries can require a much finer grid, which could lead to significantly longer run-times.
  - Is thermal required? Are chemical reactions important?
- What amount of time needs to be simulated?
  - Several time-scales could be important:
    - fluidization / hydrodynamics – how long does it take for the flow behavior to become quasi-steady?
    - thermal – in some cases, thermal transients can be quite long.
    - chemistry – is the chemistry fast or slow compared with other time-scales?
  - Usually, we want to simulate something close to “steady state”, so keep in mind how long it will likely take to reach a “steady state” based on your initial conditions.

Questions to Ask About Every Simulation You Run

- What simplifications can be made?
  - Answer this question before CAD is created. In some cases, simplifications to the geometry of the unit can significantly alter the final CAD design.
  - CAD simplifications can involve several types of simplifications
    - Exclusion of small or unimportant features
    - Making small features bigger if they must be included, to make gridding easier
    - Modeling small cylindrical features as square cross-sections for easier gridding
  - Where can the model be started and stopped? Would some boundary condition simplifications make the model much easier to set up, without sacrificing the usefulness of the results?

The "Workhorse" Model

- In many cases, you can learn more about your system by running many "coarse" models rather than a single very detailed model.
- The simplified gasifier that we will set up first is an example of such a workhorse model. It runs quickly and can be used to evaluate changes in overall operating conditions. Workhorse models are good for answering big-picture "what-if" questions, such as:
    - "What if the superficial velocity is changed?"
    - "What if the PSD of the bed is changed?"
    - "What if the system pressure is raised from 1 atm to 1.5 atm?"
- More detailed models are useful if operating conditions are already well-defined, and if smaller variations in operating conditions need to be compared.

Coarse-to-Fine Resolution Studies

- It is good practice with any CFD study, including CPFD Barracuda studies, to ensure that you have enough resolution to capture the physics of the system being simulated.
- In Barracuda, this resolution depends both on the number of computational cells and the number of computational particles.
- When running multiple simulations at different resolutions, it is best to run coarse variations first, since they will be the fastest. Then, move toward more fine-resolution cases, and compare them with the results of the already-run coarse simulations.
- This strategy allows you to identify when you have enough resolution in the shortest amount of time.

Goals for Gasifier Training Models

- Two distinct models for this training course.
- The "workhorse" model: isothermal, no chemistry, with simplifications to the geometry.
  - From this model, we want to learn:
    - General fluidization behavior
    - Estimate entrainment of particles (both rate of entrainment and PSD of entrained particles)
- The detailed model: chemistry and thermal are included, and the geometry is more realistic.
  - From this model, we want to learn:
    - Are there any thermal "hot-spots" in the bed?
    - What is the gas composition exiting the gasifier?