Tutorial 2: Spouted Bed Combustor

In this tutorial we will model a partial combustor with geometry as shown in Figure 1. Char (18 g/s) and air (10 g/s) are fed into the combustor through a central tube. A second stream of fluidizing air (116 g/s) enters the annular region surrounding the tube. Partial combustion of the char occurs in the combustor. The product gases exit from the top of the combustor. The char density is 1 g/cm^3 and the particle diameter is 1000 μm. The average void fraction in the reactor is estimated to be 0.5.

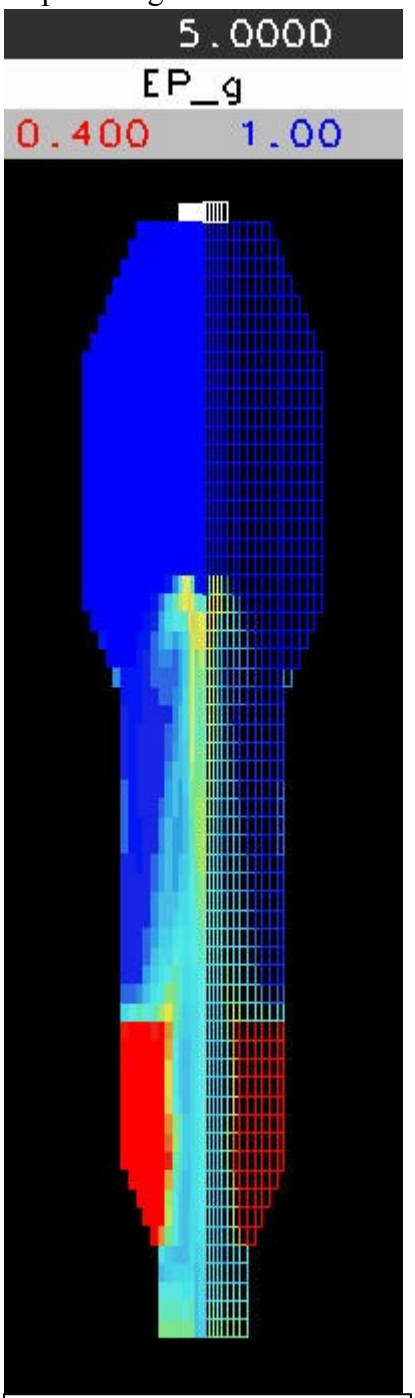

Figure 1. Geometry of the Spouted Bed Combustor

An MFIX simulation will be used to determine the characteristics of the gas-solids flow and combustion within the spouted bed combustor.

Since the incoming char is at a low temperature and it is critical to consider char heat-up, the incoming char will be treated as a second solids phase called "cold-char." The char already in the combustor will be called "hot-char." When the ash fraction in the cold chare exceeds a certain specified value, say 0.9, it is assumed to convert into hot-char. A fast pseudo-reaction is specified to convert the cold-char at temperatures above that value to hot-char. These ash fraction threshold and rate constant are specified in mfix.dat as constants C(1) and C(2), which are used in the subroutine rrates.

Four gas species are considered: 1. O_2, 2. CO, 3. CO_2, and 4. N_2. Two pseudo-species are considered in the solids phases: 1. Fixed carbon and 2. Ash. The numbering scheme shown above will be used for identifying the species in MFIX.

The chemical reactions considered are the following:

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

CO combustion: $CO + ½O_2 \rightarrow CO_2$

Gasification: $C + CO_2$ _ $2CO$

Pseudo-reaction: Cold-char → Hot-char.

1 Specifying Reaction Kinetics

The reaction rates are specified in the file *rrates.f*, which is divided into five sections. User input is required in the first four sections only. In the first section, the reaction rates for the reactions are coded (four reactions in this case). The forward and backward reactions are written separately. For specifying the rate of the pseudo reaction, we have used the user-defined constants C(1) and C(2), so that they may be entered from the data file. In the second section, the reaction rates computed in the first section are used to compute the formation and consumption rates for individual species. In the third section, the reaction rates are used to compute the mass transfer between the phases. In the fourth section, the heats of reaction are used to compute the heat generation or consumption in each of the phases. In the fifth section, certain bookkeeping and error checking computations are performed, which require no user input.

2 Writing User-Defined Subroutines

In addition to *rrates.f*, we also need to write the user-defined routines *physical_prop.f*, *usr0.f*, *usr1.f*, *usr_init_namelist.f*, and *usrnlst.inc*. In *physical_prop.f*, the gas density, gas specific heat, and solids specific heat are computed.

In *usr0.f*, the user-defined input data are checked for error and a constant is calculated based on the user-defined input. In *usr_init_namelist.f*, the two user-defined namelist variables are initialized as UNDEFINED, which is a number defined in MFIX to indicate undefined double precision numbers. By initializing values this way, the user is able to check whether the values are specified through the input file. *usrnlst.inc* file contains the definitions of user-defined variables, user-defined common blocks, and a namelist section.

3 Writing the Data File

The input data file is *mfix.dat*. In the run-control section, the energy balance calculations and species balance calculations are turned on. Since the subroutines *usr0.f* and *usr1.f* are to be used, the CALL_USR switch is turned on.

The two user-defined constants C(1) and C(2), used in the subroutine RRATES, are specified. They have been given (optional) names, with which to label them in the *.OUT* file.

In the radial direction, a nonuniform grid is used to get a better resolution near the jet. The first four radial grids are 0.5 cm wide and the next four grids expand to approach 1 cm. The last 11 grids have a size of 1 cm. The axial grid size is 2.5 cm.

The number of gas species is specified as 4 and their molecular weights are given. The number of solids phase species is specified as two. The molecular weight of ash is specified as 56. (This value, however, is not needed and is specified only to satisfy the error checker).

For simplicity, the entire domain is divided into two sections (bed and freeboard) and uniform initial conditions are specified in each section. Although this is not appropriate for the many wall-cells in the range, such an initial condition specification will not cause any problem. Also, for the central jet region, the specified void fraction is too low. The solids will clear out of that region, as the MFIX calculations progress.

There are two flow inlets and one outlet. Note that mass flows are specified instead of the axial velocity component. Also the composition of gases and solids at the inlet are specified. At the outlet only the pressure is specified.

The reactor geometry is specified with 17 obstacles. We have started the obstacles' specification as boundary condition number 20, so that any future additions or deletions of inlets or outlets can be accommodated without having to change the boundary condition indices for the obstacles.

An internal surface has been specified to simulate the central tube at the bottom of the reactor.

The keyword Report_mass_balance_dt=1 has been included to conduct an overall species mass balance check every 1 s. Use this feature only for debugging the run; for production runs disable this feature, as it slows down the simulation. To disable the feature comment out or delete the keyword (do not set it to 0 or a large value.)

The keyword nRR=7 has been included to write out seven reaction rate fields. The seven fields to be written out are chosen in the rrates routine.

The *.RES* file is written every 0.01 s and all the *.SPx* files are written every 0.1 s. Diagnostics from the code are printed out every 100^{th} time step.

4 Running MFIX

The FORTRAN files discussed in sections 1 and 2 and the input data file discussed in section 3 are stored in a run directory. To create an MFIX executable, type

make_mfix

The script file will then ask whether any user-defined files need to be copied. Type **y** to use user-defined files and specify the path name to the run directory. All the user-defined files discussed in sections 1 and 2 will be copied into the MFIX/model directory and an MFIX executable will be created and copied into the run directory.

As always, set TSTOP=0 and run MFIX. Correct any input errors until MFIX successfully reads the input data file and exits. MFIX will write all the output files. Read the *.OUT* file to verify that the inputs were read correctly. Verify that the cell flags are assigned correctly. Note how the wall cells have been assigned to approximate the

geometry of the reactor. Also note how the impermeable internal surface has been specified at the east face of the cells i=3 and j=2-6.