Running MFIX for Dummies
3dCfb case from Tutorials

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Installing MFIX

Before running MFIX for the first time, download MFIX from the member's pages of the MFIX website (http://www.mfix.org) to the directory where you want to install the code. To install the code on the computer, go to the directory in which you have downloaded the code and type:

```
gunzip -d mfix.tar.gz
tar xvf mfix.tar
```

These commands will create a directory named mfix, which contains the six subdirectories: doc, model, post_mfix, tests, tutorials, and tools.

This documentation walks you through running the Three Dimensional Circulating Fluidized-Bed (3dCfb) case, which is located in the tutorials subdirectory. Although MFIX is written in FORTRAN, no knowledge of this programming language is needed to understand this document.

To follow along with this guide to the 3dCfb case, from the home directory type:

```
mfix/tutorials/3dCfb
```

Setting up the Input File

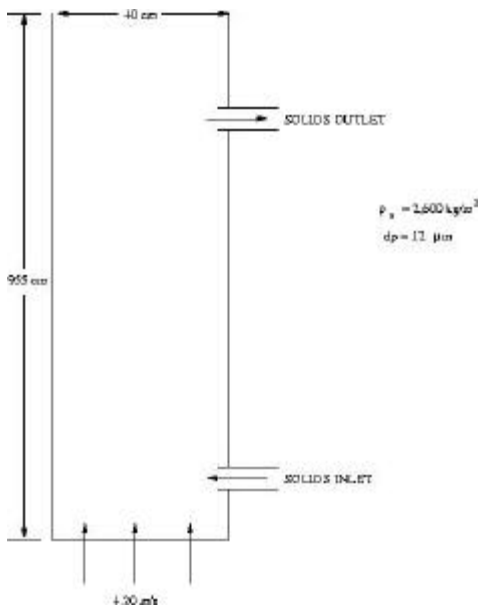


Fig. 1: Diagram of the reactor modeled by the 3dCfb case

To aid in visualizing the reactor being modeled, the mfix.dat file (located within the

3dCfb folder in the tutorials subdirectory) can be used to sketch its geometry. Any drawing program (xfig, star office, etc.) will do. The mfix.dat file may be viewed using a text editor such as vi, gedit, or nedit. The variables that can be defined in mfix.dat, are listed in a readme file (go to mfix/readme.pdf), with an explanation of their function.

The first section, called RUN CONTROL, defines parameters that control how the computer runs the code, as the term suggests. The name used to label the output files when they are created is defined as RUN_NAME and the nature of the problem addressed by this run is defined (in 60 characters or less) in DESCRIPTION. The units used for data input and output are listed in UNITS. The type of run (a new run or a previous run that is being restarted) is listed in RUN_TYPE. For the very first run of any particular simulation, the RUN_TYPE must be set to 'new'. After that, if a normal restart run is desired (with no additional user-defined changes to the restart file), RUN_TYPE should be given the value 'restart_1'. The starting and stopping times are defined in TIME and TSTOP, respectively. The starting time step is defined in DT. If this variable is not defined, a steady state calculation is performed. ENERGY_EQ controls whether or not energy equations are solved, by being set to '.TRUE.' or '.FALSE.' Similarly, the value of SPECIES_EQ controls whether or not species equations of phase m are solved. In this case, m has the value two (0- gas phase, 1- solids phase) and the '.F.' indicates that such equations are not to be solved. The value of the final variable in this section, CALL_USR, determines whether or not user-defined subroutines are called.

The PHYSICAL PARAMETERS section is rather small in this test case. The first variable (e), sets the value of the coefficient of restitution for particle collisions. The second variable (Phi), sets the value of the angle of internal friction (in degrees). Since it is set to zero, plastic regime stress calculations will not be done.

The GEOMETRY section gives the basic parameters of the reactor. The coordinate system used (either Cartesian or cylindrical) is defined as COORDINATES. In this case, “CYLINDRICAL” is selected. The width (in the length units defined in UNITS) is listed as XLENGTH. Since the geometry being considered is symmetrical, MFIX only considers one-half plane of the actual reactor and then assumes that the final geometry is obtained by rotating this plane about the axis. Thus, to calculate the actual diameter of the reactor, XLENGTH must be doubled. The number of cells in the radial (x) direction is defined as IMAX. The height of the reactor is listed as YLENGTH and the number of cells in the axial (y) direction is defined as JMAX. The reactor length in the z direction is defined as ZLENGTH and the number of cells in the z direction is defined as KMAX. In cylindrical coordinates, the z direction is the azimuthal angle.

The GAS section defines variables pertaining to the gas phase. The average molecular weight of the gas is listed in MW_avg and the specified constant gas density is defined in MU_g0.

The PARTICLE section contains the characteristics of the solids being used. The number of solids phases is defined as MMAX. Here MMAX =1, so there is only one solids phase. The particle diameter is listed in D_p. The particle density is defined in RO_s. The packed bed void fraction is defined in EP_star and the variable ur_fac(m)

stores the value of the under-relaxation parameter.

The INITIAL CONDITIONS section specifies the initial condition (IC) of a number of variables over a pie-shaped (cylindrical coordinates) or rectangular (Cartesian coordinates) region that corresponds to a numerical grid. The radial boundaries are defined by the values of X_w and X_e ("west" and "east"), the axial boundaries by Y_s and Y_n ("south" and "north"), and the z-direction boundaries by Z_b and Z_t ("bottom" and "top"). Please note that x values are listed for only one side of the reactor (due to the line of symmetry), so that the actual coordinates of the IC region are (-) IC_X_e to (+) IC_X_e. The initial void fraction in this region is stored in IC_EP_g and the initial solids pressure (usually zero) is defined as IC_P_star. The x, y, and z components of the gas velocity are stored in IC_U_g, IC_V_g, and IC_W_g, respectively. Similarly, the x,y,z components of the solids velocity are stored in IC_U_s, IC_V_s, and IC_W_s. The initial gas-phase temperature in this region is stored in IC_T_g.

The BOUNDARY CONDITIONS section lists the parameters of the air and solids inlets and the gas-solids outlet. The dimensions of the air inlet are indicated as in the IC section, by: BC_X_w, BC_X_e, BC_Y_s, BC_Y_n, BC_Z_b, and BC_Z_t. Mass inflow rates for gas and solids phases are specified at the boundary, a condition indicated by giving the value 'MI' to BC_TYPE. The void fraction, gas pressure, and gas-phase temperature in the BC plane are listed in BC_ep_g, BC_p_g, and BC_T_g, respectively. The x,y,z components of the gas velocity are listed as BC_U_g, BC_V_g, and BV_W_g. Similarly, the x and z components of the solids velocity are listed as BC_U_s and BC_W_s, while BC_MASSFLOW_s sets the value of the solids mass flow rate through the boundary. The dimensions of the solids inlet are described in the same manner as those of the air inlet. In fact, all of the variables discussed for the air inlet are present in this section. The user should take care when reading the boundary conditions section, so as not to mistake air inlet parameters for those of the solids inlet. The boundary condition dimensions of the gas-solids outlet are defined in the same manner as those of the air and solids inlets. However, the only other variables listed in this section are BC_TYPE, which is set to 'PO' to indicate outflow to a boundary at a specified pressure. This (gas-phase) pressure is stored in BC_P_g.

The OUTPUT CONTROL section contains directions for creating the output files. The interval at which the restart file (Run_Name.RES) is updated is stored in RES_DT. Similarly, the interval at which the Run_Name.SPX files are updated is stored in SPX_DT. The interval at which user-defined outputs are written from the subroutine WRITE_USR1 is stored in USR_DT. The interval (in number of time steps) at which the Run_Name.LOG file is written is stored in NLOG. Giving the final variable, FULL_LOG, the value ".TRUE." indicates that the compiler should display the residuals and messages about convergence on the screen and in the Run_Name.LOG file.

Running MFIX

To create a serial MFIX executable, go to the 3dCfb directory and type:

```
sh ../../model/make_mfix
```

The computer will prompt you to answer 4 questions. Answer *n* or press the return

key after each of them (no is the default answer).

After the successful creation of the MFIX executable (mfix.exe), it is time to run the code. To do so, you may run MFIX in the foreground or run it in the background and pipe the output to a file.
For example, you might type:

```
,/mfix.exe
        or
prun -n 1 -N 1 mfix.exe > out1 &
        or
nohup ./mfix.exe > out1 &
```

where out1 is the name of the output file (arbitrarily chosen) and the & symbol tells the computer to run the process in the background. The actual run command will vary depending on the computer being used.

While the code is running, you may check the status of the output using the tail command (type: tail -f out1). After the run has finished, you may view the entire output file using a text editor, or view the last few lines of it using tail (e.g., to view the last 100 lines, type: tail -100 out1).

Post Processing MFIX

Post processing using post_mfix can be done after MFIX has been successfully completed or anytime after the initial data files are written. Before doing post processing for the first time, an executable for post_mfix must be created. To do this, go to mfix/post_mfix and type:

```
sh make_post
```

To post process the results of 3dCfb, first open the folder and display its contents using the command *ls*. Next, access the post_mfix executable by typing its address (for example, mfix/post_mfix/post_mfix.exe).

When prompted for the run name, enter the same run name indicated when setting up the input data file. After this prompt, a menu appears with seven options. The first (0) allows the user to exit the program; number (1) is the most commonly used and is described below; number (2) and number (3) allow the user to write special restart files; number (4) allows the user to print a text file containing such quantities as granular viscosity, temperature, and time-averaged gas/solids fluxes; number (5) allows the user to print a text file with the field variables, as defined in the Run_Name.OUT file; and number (6) allows the user to access the user-defined subroutine file, if it exists. When this menu comes up, choose option 1 (Examine/Print Data). A series of prompts follows (see below). In each case, the responses are shown by the boldfaced values.

In the first line of these commands, the time range of analysis is specified.

Time: (0.000, 0.000)> **0.1, 1.0**

In the next two lines, the user specifies whether or not he wants the values to be time averaged and which variable he wishes to examine. The default variable is the void

fraction of the gas (EP_g). Alternatively, the user may wish to examine the gas or solids velocity, or any other variables written to the Run_Name.RES or Run_Name.SPX files. The gas velocity in the x,y, and z direction is represented by U_g, V_g, and W_g, respectively. For the solids velocity, just replace '_g' with '_s'.

Time average ? (N) > **Y**
Variable: (EP_g)> **[press the return key]**

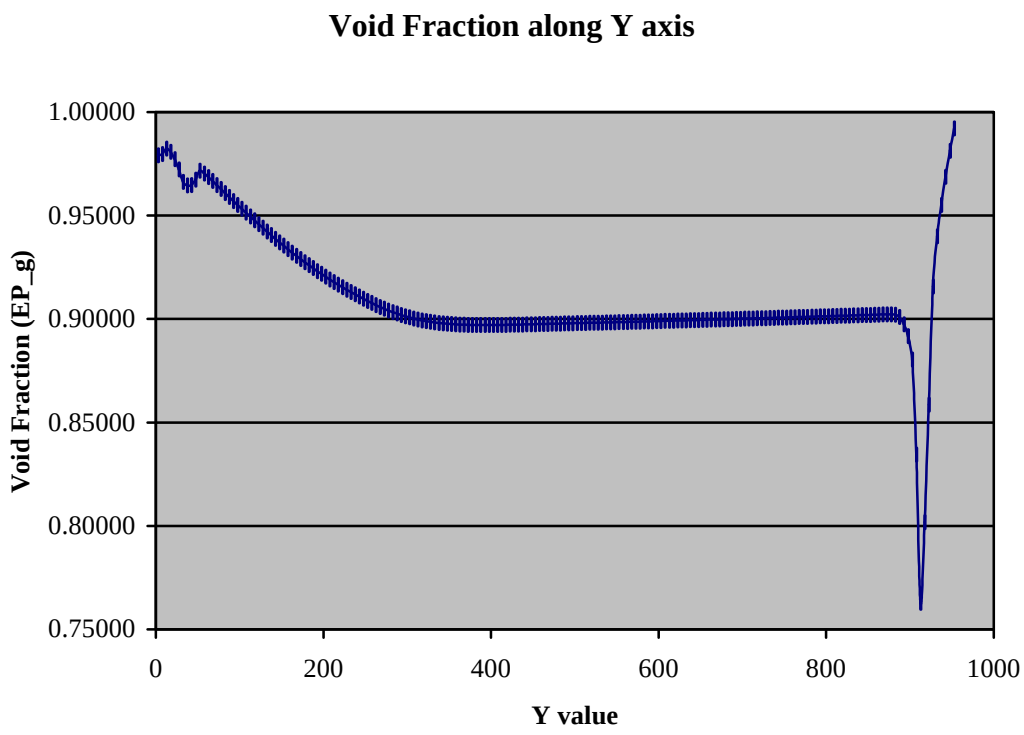
Next, the user is prompted for the range of each of the variables (I, J, K). To ensure that all of the data is incorporated, it is a good idea to initially overshoot the upper bound so that the computer will inform you what it is precisely. The desired range for each variable is: 2 to (maximum value minus 1). When asked whether to average or sum over a variable, the user should reply 'N' only to the variable along which he wishes to examine the data. For example, by answering 'N' to the J range, the user will obtain void fraction values in the axial direction. (For radially and azimuthally averaged values, the user should reply 'N' to the I range and 'Y' to J and K).

I range: (1, 1)> **2,1000**
I1 and I2 should be in the range 1 to 18
I range: (2, ****)> **2,17**
Average or sum over I? (N) > **Y**
J range: (1,1)> **2,1000**
J1 and J2 should be in the range 1 to 193
J range: (2,****)> **2,192**
Average or sum over J? (N)> **[press the return key]**
K range: (1, 1) > **2,1000**
K1 and K2 should be in the range 1 to 14
K range: (2,****)> **2,13**
Average or sum over K? (N) > **Y**

The final step is to name the data file to which the post processing output will be sent. In the example below, the file is named test-EP.dat. Once this step is completed, the user should give a negative number to go to the initial menu (and exit the program by choosing option 0) or continue filling in values for further analysis.

File: (*)> **test-EP.dat**
Time (0.100, 1.000) > **-1**

The contents of the post processing output may be viewed with a text editor. They can also be imported to a spreadsheet (such as those found in Star Office or Microsoft Excel) in order to graph the data.



Animating MFIX

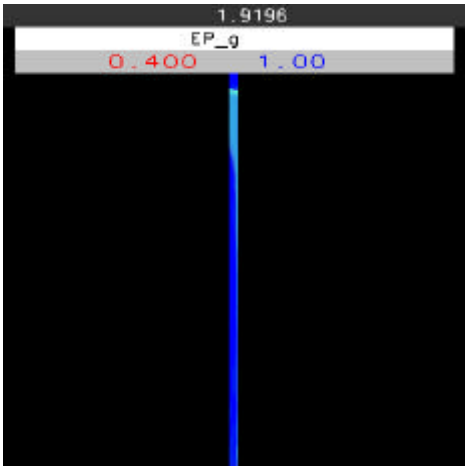
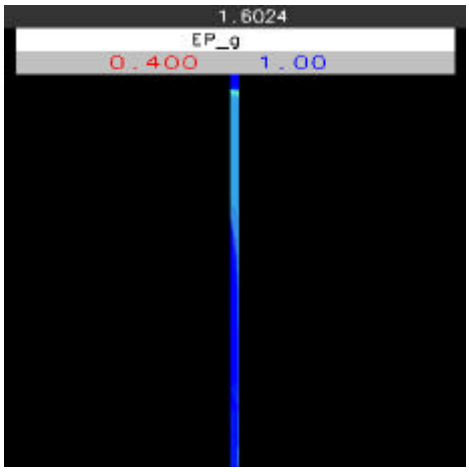
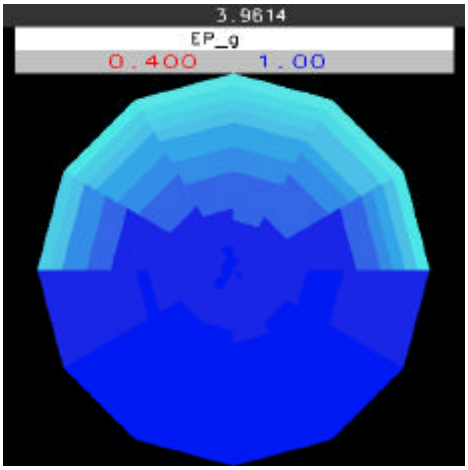
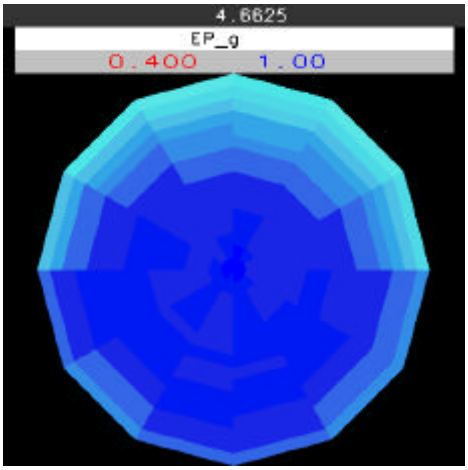
To animate the MFIX output, first obtain the animation executable (ani_mfix.exe) from the MFIX website (http://www.mfix.org). Once this is complete, and the desired case (here, it is 3dCfb) has been run or is still running with MFIX, open the folder containing the Run_Name.RES file. In this example, you would open the directory: 3dCfb. View the contents of the directory with the command *ls*. Next, access the animation executable by typing, for example:

mfix/animate_mfix/ani_mfix.exe

When prompted for the name of the restart file, enter the name exactly including the extension .RES (in this case, CFB3D.RES). Immediately, the animation window will appear.

Animate MFIX has many options. By right clicking on the graphic representation, you can change the variable being examined (the void fraction is the default) to any of the following: gas pressure, P_star, (x,y,z component of) gas or solids velocity, ROP_s, gas temperature, solids temperature, X_g, X_s, Theta_m, or scalars. Also, you can toggle the gas or solid vectors and choose between filled and lined contours. In addition, you can change the scale and the vector parameters, toggle the time averaging, and remove the plot. From the main control toolbar, you can change the x,y,z components of the image, such as viewing the animation axially or radially.

To save an image, first type *f* to freeze the screen and then type *i* to save an image as a BMP bitmap. To continue viewing the animation, left-click the window and then type *f*.

The keyboard shortcuts for this program are listed in the help menu of the main control toolbar. They are: toggle help window (h key), select plot (left mouse button), change variable and scale (right mouse button), scroll the plots (arrow keys), zoom out (x key), zoom in (z key), reset zoom/scale (r key), toggle freeze/go (f key), step a paused animation (s key), toggle automatically creating image files (m key), create image file (i key), toggle background color (b key), toggle gray/color scales (g key), select previous j/k slice (- key), select next j/k slice (+ key), select next j/k (= key), and go to script N(0-10) (1,2, … 9,0 keys).

Sample frozen animation images of 3dCfb test case: