MFIX

Multiphase Flow with Interphase eXchanges

Version MFIX-2002-3 (Date: 07/22/02)

Notice

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1 Setting Up and Running MFIX on a UNIX/LINUX Workstation

1.1 Creating MFIX Directory

To install MFIX (version m.n) from the tar file, go to the home directory and type

gunzip -d mfix.tar.gz

tar xvf mfix.tar

This procedure will create the directory mfix, which contains six subdirectories: *doc, model, post_mfix, tests, tutorials, and tools*:

Subdirectory	Contents
model	MFIX source files
post_mfix	Post_mfix source files
tutorials	Several example problems and a pdf file describing the two tutorials (fluidBed1 and fluidBed2), which are useful for a new user
tests	test simulations used to verify the code during development
tools	development tools
doc	MFIX manuals in pdf format
Complex-chemistry	An example coal gasifier case is provided dealing with complex chemistry

The postprocessing code *ani_mfix* is used to view MFIX results as animations. A linux binary is available on the download page.

1.2 Installing the MFIX Code

For convenience, create aliases by adding the following lines to the *.login* file (assuming MFIX was installed in the home directory):

```
alias ani ~/mfix/ani_mfix/ani_mfix

alias post ~/mfix/post_mfix/post_mfix

alias mkmfix >sh ~/mfix/model/make_mfix
```

Then the post-processors can be activated from any directory by typing **ani** or **post**, and the mfix make file can be activated by typing **mkmfix**.

For the first time, the user should logout and login or type: **source .login** so that the aliases are defined. This step needs to be done only once.

1.3 Starting a New Run

Create a separate subdirectory for each run.

If you want to modify MFIX subroutines, do the following. Copy the subroutine from the *mfix/model* directory into the run directory. Modify the file copied to the run directory. Do not modify the files in the *mfix/model* directory.

Create an MFIX executable file by typing **mkmfix**. The MFIX executable file *mfix.exe* will be created and copied into the run-directory.

The following options are available for different compilations:

1. For Shared Memory Executable, input >y= for the SMP option.
2. For Distributed Memory Executable , input >y= for the DMP option.
3. For Debug option, input > y= for the debug option.
4. To force recompilation of user defined routines, input >y= at this prompt. In most cases it is not necessary to select this option. This option is needed only in the rare instances when the run directory contains a module file (e.g., *run_mod.f*) and another file (e.g., *usr0.f*), in which the corresponding use statement has been inserted (e.g., use run). The makefile will not be aware of this dependency (*usr0* depends upon *run*). So, in this example, changes made in *run_mod.f* will not cause the (necessary) recompilation of *usr0.f*, unless this option is selected.

If all the above options are unselected, an optimized serial version executable is produced for that particular platform.

Write an MFIX data file and name it *mfix.dat*. The key words are listed at the end of this file. Examples are available in the *mfix/tutorials* directory.

Run MFIX by typing **mfix.exe**, or run in batch mode by typing **mfix.exe &**, or run in batch mode with the screen output redirected to a file (FULL_LOG = .TRUE. in the data file), for example, *screen.log* , by typing **mfix.exe > screen.log &**. (Note that the file *screen.log* can become very large.)

If the code was compiled as a SMP version, then you will be prompted to enter the number of processors to be used for the run.

Run the DMP version using **mpirun -np <Number of Processors> mfix.exe** . This command may be different on other machines (e.g., **mpprun -n <Number of Processors> mfix.exe**).

MFIX results can be retrieved, even while the run is in progress. To activate visualization, run *ani_mfix* by typing **ani**. When *ani_mfix* is used the first time for a run, you will be prompted for the name of the restart file. Enter the name of the restart file paying attention to the case (e.g., *BUB01.RES*).

The program will create several control files: *ani_mfix.con, ani_mfix.ini, ani_mfix.mm, script.001*.

To retrieve and manipulate data and to create special restart files, run the post_processor *post_mfix* by typing **post**. *post_mfix* will prompt the user for the run name. Enter the run name (e.g., *BUB01*).

1.4 Modifying the Post-Processing Codes

To make *post_mfix*, first change the directory to the *mfix/post_mfix* directory. If user-defined post-processing is required, modify the *usr_post.f* file in the directory. Then type **make_post**. Note that the *mfix/model* is required for creating a *post_mfix* executable.

2 Setting Up and Running MFIX on a PC (Windows 95/98/NT)

2.1 Installing the MFIX Code

This is not very well supported and please see our download page for special remarks and also earlier postings on mfix-help mailing list.

3 MFIX at Run Time

3.1 MFIX Output and Messages

MFIX output is stored in nine **.SPx* binary files. The restart info is periodically written to the **.RES* binary file. The text file **.OUT* echos the input, shows the numerical cell distribution, and, if OUT_DT is defined, prints the field variables at the specified intervals.

The text file **.LOG* contains run information. For the DMP version, a LOG file is created for each of the processors and they are numbered as *Name###.LOG*.

Messages about the run are written to the *.LOG* file. The progress of the run will be displayed at the terminal as shown below if the data file specifies FULL_LOG = .TRUE.

Time = 0.92965 Dt = 0.13930E-02 CPU time left = 54.672 s

Nit	P0	P1	U0	V0	U1	V1	Max Res
1	1.5E-02	2.5E+01	1.3E-03	3.3E-03	3.2E-03	6.3E-03	P0
2	1.	5.0E-02	2.8E-03	6.3E-03	2.5E-03	3.8E-03	P1
3	0.1	2.1E-02	1.2E-03	3.7E-03	1.1E-03	1.8E-03	P0
4	5.2E-02	8.1E-03	6.5E-04	2.1E-03	4.8E-04	8.6E-04	P0
5	3.0E-02	3.9E-03	4.1E-04	1.3E-03	2.5E-04	4.3E-04	P0

The first line shows the time, the time-step, and the CPU time remaining to complete the run. The CPU time remaining is not accurate, especially in the beginning of the run. For each time-step, the normalized residuals for various equations are written out every iteration.

MFIX uses a variable time step, which is automatically adjusted within user-defined limits to reduce the run time. At large values of Dt, the iterations may not converge. When this happens, the time step size is successively reduced until convergence is obtained. Messages about divergence and recovery are displayed on the terminal and in the *.LOG* file, if FULL_LOG = .TRUE.

The subsequent lines display the iteration number, the normalized residuals for various equations (e.g., gas continuity, solids continuity, x and y gas momentum, and x and y solids momentum), and the equation with the maximum residual. The residuals P0 and P1 are normalized only when Nit>1. The residuals displayed can be selected with the keyword RESID_STRING.

MFIX reports errors while reading the data file, while processing input data, and during the run time. Errors in reading the data file and in opening files are reported to the terminal. All other errors are reported in the *.LOG* file.

While reporting errors in reading the data file, MFIX displays the offending line of input, so that the error can be easily detected. The possible causes of error are (1) incorrect format for the name-list input, (2) unknown (misspelt) variable name, or (3) the dimension of the name-list item is too small. For example, if the dimension of DX is set as 5000 (DIM_I in *param_mod.f*), and if the input data file contains an entry DX(5001), MFIX will report an input processing error.

While processing the input data, MFIX will report errors if the data specified is insufficient or physically unrealistic. MFIX will supply default values only when it is certain that giving a default value is reasonable.

An occasional input-processing error is the inability to determine the flow plane for a boundary condition. The boundary planes defined in the input data file must have a wall-cell on one side and a fluid-cell on the other side. If the initial condition is not specified for the fluid-cell, MFIX will not recognize the cell as a fluid-cell and, hence, MFIX will be unable to determine the flow plane.

Every NLOG (see Appendix) number of time steps, MFIX monitors whether the mass fractions add up to 1.0; the overall reaction rates add up to zero; the viscosities, conductivities, and specific heats are greater than zero; and the temperatures are within the specified limits. A message will be printed out if any errors are encountered. The run may be aborted depending upon the severity of the error. Every NLOG time step, MFIX will print out the number of iterations during the previous time step and the total solids inventory in the reactor.

For the specified mass-outflow condition, after the elapse of time BC_DT_0, MFIX prints out time-averaged mass flow rates. For cyclic boundary conditions, MFIX will print out the volume averaged mass fluxes every NLOG time step.

A message is written to the *.LOG* file whenever the *.RES* and *.SPx* files are written. This message also shows an approximate value of the cumulative disk space usage in megabytes.

3.2 Restarting a Run

A run is restarted by rerunning MFIX after typing RUN_TYPE = 'restart_1' in *mfix.dat*. The old *.OUT* file will be overwritten. The *.LOG* messages will be appended to the old *.LOG* file.

There are three other types of restarts; refer to the Appendix for details.

3.3 When the Run Does Not Converge

Initial non-convergence: Ensure that the initial conditions are physically realistic. If in the initial time step, the run displays NaN (Not-a-Number) for any residual, reduce the initial time step, since automatic time step reduction will become ineffective. If time step reductions do not help, recheck the problem setup.

Holding the time step constant (DT_FAC=1) and ignoring the stalling of iterations (DETECT_STALL=.FALSE.) may help in overcoming initial nonconvergence. Often a better initial condition will aid convergence. For example, using a hydrostatic rather than a uniform pressure distribution as the initial condition will aid convergence in fluidized-bed simulations.

If there are computational regions where the solids tend to compact (i.e., solids volume fraction less than EP_star), the convergence can be improved by reducing UR_FAC(2) below the default value of 0.5.

Convergence is often difficult with higher order discretization methods. First order upwinding may be used to overcome initial transients and then the higher order method may be turned on. Also, higher-order methods such as van Leer and minmod give faster convergence than methods such as superbee and ULTRA-QUICK.

4 Keywords in Input Data File (*mfix.dat*)

[ ] indicates the default value.

The symbols used in the table are as follows:

Dimension	**Description**	**Type**	**Description**
1	Cell number in x, y, or z direction	C	Character
m	Solids-phase number	DP	Double Precision
n	Species number	I	Integer
ic	Initial condition number	L	Logical
bc	Boundary condition number		
is	Internal surface number		
usr	User-defined output number		

4.1 Run Control

Keyword (dimension)	Type	Description
RUN_NAME	C	Name used to create output files. The name should be legal after extensions are added to it; e.g., for run name BUB01, the output files BUB01.LOG, BUB01.OUT, BUB01.RES, etc., will be created.
DESCRIPTION	C	Problem description in 60 characters.
UNITS	C	Units for data input and output.
[CGS]		All input and output in CGS units.
RUN_TYPE	C	Type of run.
NEW		New run.
RESTART_1		Normal restart run. Initial conditions from .RES file.
RESTART_2		Start a new run with initial conditions from a .RES file created from another run.
RESTART_3		Continue old run as in RESTART_1, but any input data not given in mfix.dat is read from the .RES file.
RESTART_4		Start a new run as in RESTART_2, but any input data not given in mfix.dat is read from the .RES file.
TIME	DP	Start-time of the run.
TSTOP	DP	Stop-time of the run.
DT	DP	Starting time step. If DT is not defined, a steady-state calculation will be performed.
DT_MAX [1.0]	DP	Maximum time step.
DT_MIN [1E-6]	DP	Minimum time step.
DT_FAC [0.9]	DP	Factor for adjusting time step. Should be less than 1. Use a value of 1 to hold the time step constant.
DETECT_STALL	L	
[.TRUE.]		Reduce time step if the residuals sum does not decrease.
.FALSE.		Do not reduce time step for stalled iterations.
MODEL_B	L	Momentum equations.
[.FALSE.]		Model A

.TRUE.		Model B
MOMENTUM_X_EQ(m)	L	(m=0 indicates gas phase)
[.TRUE.]		Solve X-momentum equations of phase m.
.FALSE.		Do not solve X-momentum equations of phase m. Beware of inconsistencies when the momentum equations are turned off; e.g., 2-D developing flow with only Y-momentum should not specify no-slip-walls.
MOMENTUM_Y_EQ(m)	L	(m=0 indicates gas phase)
[.TRUE.]		Solve Y-momentum equations of phase m.
.FALSE.		Do not solve Y-momentum equations of phase m.
MOMENTUM_Z_EQ(m)	L	(m=0 indicates gas phase)
[.TRUE.]		Solve Z-momentum equations of phase m.
.FALSE.		Do not solve Z-momentum equations of phase m.
ENERGY_EQ	L	
[.TRUE.]		Solve energy equations
.FALSE.		So not solve energy euqations
SPECIES_EQ(m)	L	(m=0 indicates gas phase)
[.TRUE.]		Solve species equations of phase m.
.FALSE.		Do not solve species equations of phase m.
GRANULAR_ENERGY [.FALSE.]	L	Use the granular energy transport equation (pde) as opposed to the algebraic (alg) equation formulation.
FRICTION [.FALSE.]	L	Use the Schaeffer model when .FALSE., or use the Princeton model when .TRUE.

The combination of the keywords GRANULAR_ENERGY and FRICTION invokes different solids stress models as shown below:

GRANULAR_ENERGY = .FALSE.

EP_g < EP_star > Schaeffer

EP_g >= EP_star > viscous (algebraic)

GRANULAR_ENERGY = .TRUE.

FRICTION = .TRUE.

EP_s(IJK,M) > EPS_f_min > Princeton + viscous (pde)

EP_s(IJK,M) < EP_f_min > viscous (pde)

FRICTION = .FALSE.

EP_g < EP_star > Schaeffer + viscous (pde)

EP_g >= EP_star > viscous (pde)

Keyword (dimension)	Type	Description
SAVAGE	I	For a term appearing in the frictional stress model invoked with FRICTION = .TRUE.
0		Use S:S in the frictional stress model.
[1]		Use an alternate form suggested by Savage.
2		An appropriate combination of the above two forms.
Nscalar [0]	I	Number of scalar equations to be solved.
Phase4Scalar(n)	I	The index of the phase that convects scalar n. Use 0 for gas phase; e.g., Phase4Scalar(3)=0 means Scalar no. 3 will be convected by gas phase.
CALL_USR	L	
.TRUE.		Call user-defined subroutines.
[.FALSE.]		Do not call user-defined subroutines.

4.2 Physical and Numerical Parameters

Keyword (dimension)	Type	Description
C(100)	DP	User defined constants.
C_NAME(100)	C	Name of user-defined constants (20 characters long). These character strings are used only to identify user-defined constants (c) in the .OUT file.
C_e	DP	Coefficient of restitution for particle-particle collisions. (MFIX 1.94 keyword _e_).

e_w [1.0]	DP	Coefficient of restitution for particle-wall collisions.
PHIP [0.6]	DP	Specularity coefficient associated with particle-wall collisions.
C_f	DP	Coefficient of friction between the particles of two solids phases.
Phi	DP	Angle of internal friction (in degrees). Set this value to zero to turn off plastic regime stress calculations.
L_scale0 [0.0]	DP	Value of turbulent length initialized. This may be overwritten in specific regions with the keyword IC_L_scale.
Mu_gmax	DP	Maximum value of the turbulent viscosity of the fluid.
V_ex	DP	Excluded volume in Boyle-Massoudi stress.
[0.0]		B-M stress is turned off.
P_ref [0.0]	DP	Reference pressure.
P_scale [1.0]	DP	Scale factor for pressure.
GRAVITY	DP	Gravitational acceleration.
[980.7]		By default, the gravity force acts in the _ve y-direction. Modify file b_force2.inc to change the body force term.
MAX_NIT [500]	I	Maximum number of iterations.
NORM_g [Use the residual from the first iteration.]	DP	Factor to normalize the gas continuity equation residual.
NORM_s [Use the residual from the first iteration.]	DP	Factor to normalize the solids continuity equation residual.
TOL_RESID [1E-3]	DP	Maximum residual at convergence (continuity+momentum).
TOL_RESID_T [1E-4]	DP	Maximum residual at convergence (energy).

TOL_RESID_X [1E-4]	DP	Maximum residual at convergence (species balance).
TOL_RESID_Scalar [1E-4]	DP	Maximum residual at convergence (scalar balances.)
TOL_DIVERGE [1E+4]	DP	Minimum residual for declaring divergence. When the fluid is incompressible, the velocity residuals take large values in the second iteration (e.g., 1E+8) and then drop down to a low value in the third iteration (e.g., 0.1). In such cases, it is desirable to increase this setting.

The next keywords LEQ_IT, LEQ_METHOD, LEQ_SWEEP, LEQ_TOL, UR_FAC, and DISCRETIZE are dimensioned for the nine types of equations:

Index	Equation Type
1	gas pressure
2	solids volume fraction
3	gas and solids v-momentum
5	gas and solids w-momentum
6	temperature
7	species mass fractions
8	granular temperature
9	user-defined scalar

For example, LEQ_IT(3) = 10 will make MFIX use 10 linear equation iterations while solving the gas and solids u-momentum equation (Equation Type =3).

Keyword (dimension)	**Type**	**Description**
LEQ_IT(9) [20 for 1 and 2] [5 for 2-5] [15 for 6-9]	I	Number of iterations in the linear equation solver. The nine values are for the nine types of equations noted above. The same convention holds for LEQ_METHOD, UR_FAC, and DISCRETIZE. If the residual of an equation is less than the convergence criterion, MFIX makes LEQ_IT equal to the lesser of 5 and the user-defined value and LEQ_METHOD equal to 1.

LEQ_METHOD(9) [1 for all equations]	I	The method used in the linear equation solver: 1. BiCGSTAB.
LEQ_SWEEP(9) [RSRS]	C	The sweep direction used in the linear equation solver. The sweep direction for preconditioning line relaxation; e.g., if LEQ_SWEEP = "ISIS", 1 sweep with do IK loop followed by send_recv (repeated twice), or if LEQ_SWEEP = "RSRS",1 red-black sweep with do IK loop followed by send_recv (repeated twice) . Only used by BiCGSTAB.
LEQ_TOL(9) [1.0D-4]	DP	The tolerance, if used, in linear equation solvers. Only used by BiCGSTAB.
LEQ_PC [LINE]	C	The preconditioner used for the sweeps in the linear solver LINE - Line relaxation DIAG - Diagonal Scaling NONE - No preconditioner
UR_FAC(9) [0.8 for 1, 6, 9] [0.5 for 2, 3, 4, 5, 8] [0.75 for 7]	I	Under relaxation factors for seven types of equations. Reducing UR_FAC(2) will help convergence in problems in which the solids tend to pack.
DEF_COR [.TRUE.]	L	If true, use deferred correction method for implementing higher order discretization. Otherwise, use down-wind factor method (default).
DISCRETIZE(9)	I	Discretization scheme for seven types of equations.
[0]		First-order upwinding.
1		First-order upwinding (using down-wind factors).
2		Superbee (recommended method).
3		SMART.
4		ULTRA-QUICK.
5		QUICKEST (does not work).
6		MUSCL.
7		van Leer.
8		Minmod.

4.3 Geometry and Discretization

For 2D simulations, the thickness of the third direction specified should be exact if mass or volumetric flow rates, rather than velocities, are specified at the boundaries.

Keyword (dimension)	Type	Description
COORDINATES	C	Coordinates used in the simulation.
CARTESIAN		Cartesian coordinates.
CYLINDRICAL		Cylindrical coordinates.
NO_I	L	(Do not use.)
[.FALSE.]		X (r) direction is considered.
.TRUE.		X (r) direction is not considered.
IMAX	I	Number of cells in the x (r) direction.
DX (l)	DP	Cell sizes in the x (r) direction. (Use uniform mesh size with second-order discretization methods.)
XMIN	DP	The inner radius in the simulation of an annular cylindrical region.
XLENGTH	DP	Reactor length in the x (r) direction.
NO_J	L	(Do not use.)
[.FALSE]		y direction is considered.
.TRUE.		y direction is not considered.
JMAX	I	Number of cells in the y direction.
DY (1)	DP	Cell sizes in the y direction. (Use uniform mesh size with second-order discretization methods.)
YLENGTH	DP	Reactor length in the y direction.
NO_K	L	
[.FALSE.]		z ( ) direction is considered.
.TRUE.		z ( ) direction is not considered.
KMAX	I	Number of cells in the z ( ) direction.
DZ (1)	DP	Cell sizes in the z ( ) direction. (Use uniform mesh size with second-order discretization methods.)
ZLENGTH	DP	Reactor length in the z ( ) direction.
CYCLIC_X	L	Flag for making the x-direction cyclic without pressure drop. No other boundary conditions for the x-direction should be specified.

[.FALSE.]		No cyclic condition at X-boundary.
.TRUE.		Cyclic condition at X-boundary.
CYCLIC_X_PD	L	Flag for making the x-direction cyclic with pressure drop. No other boundary conditions for the x-direction should be specified.
[.FALSE.]		No cyclic condition at X-boundary.
.TRUE.		Cyclic condition with pressure drop at X-boundary.
DELP_X	DP	Fluid pressure drop across XLENGTH when a cyclic boundary condition with pressure drop is imposed in the x-direction.
CYCLIC_Y	L	Flag for making the y-direction cyclic without pressure drop. No other boundary conditions for the y-direction should be specified.
[.FALSE.]		No cyclic condition at Y-boundary.
.TRUE.		Cyclic condition at X-boundary.
CYCLIC_Y_PD	L	Flag for making the y-direction cyclic with pressure drop. No other boundary conditions for the y-direction should be specified.
[.FALSE.]		No cyclic condition at Y-boundary.
.TRUE.		Cyclic condition with pressure drop at Y-boundary.
DELP_Y	DP	Fluid pressure drop across YLENGTH when a cyclic boundary condition with pressure drop is imposed in the y-direction.
CYCLIC_Z	L	Flag for making the z-direction cyclic without pressure drop. No other boundary conditions for the z-direction should be specified.
[.FALSE.]		No cyclic condition at Z-boundary.
.TRUE.		Cyclic condition at Z-boundary.
CYCLIC_Z_PD	L	Flag for making the z-direction cyclic with pressure drop. No other boundary conditions for the z-direction should be specified.
[.FALSE.]		No cyclic condition at Z-boundary.
.TRUE.		Cyclic condition with pressure drop at Z-boundary.
DELP_Z	DP	Fluid pressure drop across ZLENGTH when a cyclic boundary condition with pressure drop is imposed in the z-direction.

SHEAR	L	If .TRUE. imposes a mean shear on the flow field as a linear function of _x_ coordinate. This feature should only be used when CYCLIC_X=.TRUE. Also, the keyword V-sh needs to be set.
V_sh	DP	Specifies the mean _y_ velocity component at the eastern boundary of the domain (V_sh), and the mean _y_ velocity (-V_sh) at the western boundary of the domain.

4.4 Gas Phase

Keyword (dimension)	Type	Description
RO_g0	DP	Specified constant gas density. This value may be set to zero to make the drag zero and to simulate granular flow in a vacuum.
MU_g0	DP	Specified constant gas viscosity.
K_g0	DP	Specified constant gas conductivity.
C_pg0	DP	Specified constant gas specific heat.
DIF_g0	DP	Specified constant gas diffusivity.
MW_AVG	DP	Average molecular weight of gas.
MW_g (n)	DP	Molecular weight of gas species n.

4.5 Solids Phase

Keyword (dimension)	Type	Description
MMAX	I	Number of solids phases.
D_p (m)	DP	Particle diameters.
RO_s (m)	DP	Particle densities.
NMAX (m)	I	Number of species in phase m. Note that m=0 indicates gas phase.
MU_s0	DP	Specified constant granular viscosity. If this value is specified, then the kinetic theory calculation is turned off and P_s = 0 and Lambda_s = -2/3 MU_s0.
K_s0	DP	Specified constant solids conductivity.

C_ps0	DP	Specified constant solids specific heat.
DIF_s0	DP	Specified constant solids diffusivity.
MW_s (m,n)	DP	Molecular weight of solids phase-m, species n.
EP_star	DP	Packed bed void fraction.
CLOSE_PACKED (m) [.TRUE.]	L	Indiates whether the solids phase forms a packed bed with a void fraction EP_star.

4.6 Initial Conditions

Each initial condition (IC) is specified over a rectangular region (or pie-shaped for cylindrical coordinates) that corresponds to the scalar numerical grid. These are 3D regions: X_w X_e, Y_s Y_n, and Z_t Z_b. The region is defined by the constant coordinates of each of the six faces, which may be specified as the physical coordinates or the cell indices. The

physical coordinates are easier to specify than the cell indices. If cell sizes are not small enough to resolve a region specified using physical coordinates, MFIX will indicate this problem with an error message.

In cylindrical coordinates, when the theta direction crosses the 0 value, split that region into two regions: e.g., Split a region spanning 1.9 pi to 0.1 pi as 1.9 pi to 2 pi and 0 to 0.1 pi.

Two initial condition regions may overlap. When an overlap occurs, MFIX uses the conditions specified for the higher IC number.

Keyword (dimension)	**Type**	**Description**
IC_X_w (ic)	DP	x coordinate of the west face.
IC_X_e (ic)	DP	x coordinate of the east face.
IC_Y_s (ic)	DP	y coordinate of the south face.
IC_Y_n (ic)	DP	y coordinate of the north face.
IC_Z_b (ic)	DP	z coordinate of the bottom face.
IC_Z_t (ic)	DP	z coordinate of the top face.
IC_I_w (ic)	I	i index of the west-most wall.
IC_I_e (ic)	I	i index of the east-most wall.
IC_J_s (ic)	I	j index of the south-most wall.
IC_J_n (ic)	I	j index of the north-most wall.
IC_K_b (ic)	I	k index of the bottom-most wall.
IC_K_t (ic)	I	k index of the top-most wall.

IC_TYPE (ic)	C	Type of initial condition. Mainly used in restart runs to overwrite values read from the .RES file by specifying it as _PATCH_. The user needs to be careful when using the _PATCH_ option, since the values from the .RES file are overwritten and no error checking is done for the patched values.
IC_EP_g (ic)	DP	Initial void fraction in the IC region.
IC_P_g (ic)	DP	Initial gas pressure in the IC region. If this quantity is not specified, MFIX will set up a hydrostatic pressure profile, which varies only in the y-direction.
IC_P_star (ic)	DP	Initial solids pressure in the IC region. Usually, this value is specified as zero.
IC_L_scale (ic)	DP	Turbulence length scale in the IC region.
IC_ROP_s (ic, m)	DP	Initial macroscopic density of solids phase-m in the IC region.
IC_T_g (ic)	DP	Initial gas phase temperature in the IC region.
IC_T_s (ic, m)	DP	Initial solids phase-m temperature in the IC region.
IC_Theta_m (ic, m)	DP	Initial solids phase-m granular temperature in the IC region.
IC_GAMA_Rg (ic) [0]	DP	Gas phase radiation coefficient in the IC region. Modify file radtn2.inc to change the source term.
IC_T_Rg (ic)	DP	Gas phase radiation temperature in the IC region.
IC_GAMA_Rs (ic, m) [0]	DP	Solids phase-m radiation coefficient in the IC region. Modify file radtn2.inc to change the source term.
IC_T_Rs (ic, m)	DP	Solids phase-m radiation temperature in the IC region.
IC_U_g (ic)	DP	Initial x-component of gas velocity in the IC region.
IC_U_s (ic, m)	DP	Initial x-component of solids-phase velocity in the IC region.
IC_V_g (ic)	DP	Initial y-component of gas velocity in the IC region.
IC_V_s (ic, m)	DP	Initial y-component of solids-phase velocity in the IC region.
IC_W_g (ic)	DP	Initial z-component of gas velocity in the IC region.
IC_W_s (ic, m)	DP	Initial z-component of solids-phase velocity in the IC region
IC_X_g (ic, n) [0]	DP	Initial mass fraction of gas species n.

IC_X_s (ic, m, n) [0]	DP	Initial mass fraction of solids phase-m, species n.
IC_SOLAR (ic, n) [0]	DP	Initial value of Scalar n.

4.7 Boundary Conditions

Boundary conditions (BC) are specified over flow planes or 2D surfaces that are normal to one of the coordinate directions and coincide with a face of the scalar control-volume. The values for one of the three pairs of coordinates are equal. The surface is defined by the constant coordinates of each of the four edges, which can be specified with physical coordinates or cell indices, and the two equal values for the direction normal to the face, which can only be specified with physical coordinates. If cell sizes are not small enough to resolve a surface specified using physical coordinates, MFIX will indicate this problem with an error message.

A flow plane must have a wall cell (or an outside boundary) on one side and a flow cell on the other side.

The BC section is also used to specify obstacles in the flow domain. Obstacles are 3D regions, just as for the IC regions: X_w X_e, Y_s Y_n, and Z_t Z_b. By default the outside boundary is initialized as no-slip walls. For cylindrical coordinates the axis is initialized as a free-slip wall.

Two boundary surfaces must not intersect. Two obstacle regions may intersect.

Keyword (dimension)	**Type**	**Description**
BC_X_w (bc)	DP	x coordinate of the west face or edge.
BC_X_e (bc)	DP	x coordinate of the east face or edge.
BC_Y_s (bc)	DP	y coordinate of the south face or edge.
BC_Y_n (bc)	DP	y coordinate of the north face or edge.
BC_Z_b (bc)	DP	z coordinate of the bottom face or edge.
BC_Z_t (bc)	DP	z coordinate of the top face or edge.
BC_I_w (bc)	I	i index of the west-most cell.
BC_I_e (bc)	I	i index of the east-most cell.
BC_J_s (bc)	I	i index of the south-most cell.
BC_J_n (bc)	I	i index of the north-most cell.
BC_K_b (bc)	I	i index of the bottom-most cell.
BC_K_t (bc)	I	i index of the top-most cell.

BC_TYPE (bc)	C	Type of boundary:
DUMMY		The specified boundary condition is ignored. This is useful for turning off some boundary conditions without having to delete them from the file.
MASS_INFLOW or MI		Mass inflow rates for gas and solids phases are specified at the boundary.
MASS_OUTFLOW or MO		The specified values of gas and solids mass outflow rates at the boundary are maintained, approximately. This condition should be used sparingly for minor outflows, when the bulk of the outflow is occurring through other constant pressure outflow boundaries.
P_INFLOW or PI		Inflow from a boundary at a specified constant pressure. To specify as the west, south, or bottom end of the computational region, add a layer of wall cells to the west, south, or bottom of the PI cells.
P_OUTFLOW or PO		Outflow to a boundary at a specified constant pressure. To specify as the west, south, or bottom end of the computational region, add a layer of wall cells to the west, south, or bottom of the PO cells.
FREE_SLIP_WALL or FSW		Velocity gradients at the wall vanish. If BC_JJ_PS is equal to 1, Johnson-Jackson bc is used for solids.
NO_SLIP_WALL or NSW		All components of the velocity vanish at the wall. If BC_JJ_PS is equal to 1, Johnson-Jackson bc is used for solids.
PAR_SLIP_WALL or PSW		Partial slip at the wall implemented as dv/dn + hw (v _ vw) = 0, where n is the normal pointing from the fluid into the wall. The coefficients hw and vw should be specified. Hw = 0 => free slip; hw = ∞ ; and vw => 0 . no slip. To set hw = oo, leave it unspecified. If BC_JJ_PS is equal to 1, Johnson-Jackson boundary condition is used for solids.

Specifications for WALL boundary conditions:

Keyword (dimension)	**Type**	**Description**

Momentum Equation		Partial slip at the wall implemented as dv/dn + hw (v _ vw) = 0, where n is the normal pointing from the fluid into the wall. The coefficients hw and vw should be specified. Hw = 0 => free slip; hw = ∞ ; and vw => 0 . no slip. To set hw = oo, leave it unspecified.
BC_hw_g (bc) [∞]	DP	Gas phase hw for partial slip boundary.
BC_hw_s (bc, m) [∞]	DP	Solids phase hw for partial slip boundary.
BC_Uw_g (bc)	DP	Gas phase Uw for partial slip boundary.
BC_Uw_s (bc, m)	DP	Solids phase Uw for partial slip boundary.
BC_Vw_g (bc)	DP	Gas phase Vw for partial slip boundary.
BC_Vw_s (bc, m)	DP	Solids phase Vw for partial slip boundary.
BC_Ww_g (bc)	DP	Gas phase Ww for partial slip boundary.
BC_Ww_s (bc, m)	DP	Solids phase Ww for partial slip boundary.
BC_JJ_PS (bc)	I	1: Use Johnson and Jackson partial slip bc. 0: Do not use Johnson and Jackson partial slip bc.
[0]		If granular energy transport equation is not solved.
[1]		If granular energy transport equation is solved.
Granular Energy Equation		The granular energy boundary condition is implemented as dT/dn + hw (T _ Tw) = c, where n is the normal pointing from the fluid into the wall. If Johnson and Jackson partial slip bc is used, the coefficients hw and c are calculated. Otherwise, they must be specified. Hw = 0 => specified heat flux; hw = ∞ => specified temperature boundary condition. To set hw = ∞ , leave it unspecified and give a value for Tw.
BC_Thetaw_m (bc, m)	DP	Tw for granular energy bc.
BC_hw_Theta_m (bc, m) [∞]	DP	Hw for granular energy bc.
BC_C_Theta_m (bc, m)	DP	c for granular energy bc.

Gas and Solids Energy Equations		The thermal boundary condition implemented as dT/dn + hw (T _ Tw) = c, where n is the normal pointing from the fluid into the wall. The coefficients hw, Tw, and c should be specified. Hw = 0 => specified heat flux; hw = ∞ => specified temperature boundary condition. To set hw = ∞ , leave it unspecified and give a value for Tw.
BC_hw_T_g (bc) [∞]	DP	Gas phase hw for heat transfer.
BC_hw_T_s (bc, m) [∞]	DP	Solids phase hw for heat transfer.
BC_Tw_g (bc)	DP	Gas phase Tw for heat transfer.
BC_Tw_s (bc, m)	DP	Solids phase Tw for heat transfer.
BC_C_T_g (bc)	DP	Gas phase C for heat transfer.
BC_C_T_s (bc, m)	DP	Solids phase C for heat transfer.
Gas and Solids Species Equations		The species diffusion boundary condition is implemented as dX/dn + hw (X _ Xw) = c, where n is the normal pointing from the fluid into the wall. The coefficients hw, Xw, and c should be specified. Hw = 0 => specified species diffusion flux; hw = ∞ => specified species concentration at the boundary. To set hw = ∞ , leave it unspecified and give a value for Xw.
BC_hwX_g (bc, n) [∞]	DP	The species diffusion boundary condition is implemented as dX/dn + hw (X _ Xw) = c, where n is the normal pointing from the fluid into the wall. The coefficients hw, Xw, and c should be specified. Hw = 0 => specified species diffusion flux; hw = ∞ => specified species concentration at the boundary. To set hw = ∞ , leave it unspecified and give a value for Xw. Gas phase hw for mass transfer.
BC_hw_X_s (bc, m, n) [∞]	DP	Solids phase hw for mass transfer.
BC_Xw_g (bc, n)	DP	Gas phase Xw for mass transfer.
BC_Xw_s (bc, m, n)	DP	Solids phase Xw for mass transfer.

BC_C_X_g (bc, n)	DP	Gas phase C for mass transfer.
BC_C_X_s (bc, m, n)	DP	Solids phase C for mass transfer.
Scalar Transport Equations		The scalar boundary condition is implemented as dS/dn + hw (S _ Sw) = C, where n is the normal pointing from the fluid into the wall. The coefficients hw, Sw, and c should be specified. Hw = 0 => specified species diffusion flux; hw = ∞ => specified species concentration at the boundary. To set hw = ∞ , leave it unspecified and give a value for Sw.
BC_hw_Scalar (bc, n) [∞]	DP	hw for scalar transfer at the boundary.
BC_ScalarW (bc, n)	DP	Xw for scalar transfer at the boundary.
BC_C_Scalar (bc, n)	DP	C for scalar transfer at the boundary.

Specifications for FLOW boundary conditions:

Keyword (dimension)	Type	Description
BC_EP_g (bc)	DP	Void fraction at the BC plane.
BC_P_g (bc)	DP	Gas pressure at the BC plane.
BC_ROP_s (bc, m)	DP	Macroscopic density of solids phase at the BC plane.
BC_T_g (bc)	DP	Gas phase temperature at the BC plane.
BC_T_s (bc, m)	DP	Solids phase-m temperature at the BC plane.
BC_Theta_m (bc, m)	DP	Solids phase-m granular temperature at the BC plane.
BC_X_g (bc, n) [0]	DP	Mass fraction of gas species n at the BC plane.
BC_X_s (bc, m, n) [0]	DP	Mass fraction of solids phase-m, species n at the BC plane.
BC_U_g (bc)	DP	x-component of gas velocity at the BC plane.
BC_U_s (bc, m)	DP	x-component of solids-phase velocity at the BC plane.
BC_V_g (bc)	DP	y-component of gas velocity at the BC plane.
BC_V_s (bc, m)	DP	y-component of solids-phase velocity at the BC plane.
BC_W_g (bc)	DP	z-component of gas velocity at the BC plane.

BC_W_s (bc, m)	DP	z-component of solids-phase velocity at the BC plane.

For a mass inflow boundary, instead of specifying the normal velocity at a boundary, the gas and solids flow rates may be specified as the volumetric or mass flow rates. If the volumetric or mass flow rate is specified, MFIX will calculate the velocity normal to the boundary. The velocity calculated by MFIX, however, may differ from the velocity calculated based on the physical dimensions of the port because the simulated dimensions may not be exactly equal to the physical dimensions. Specify positive values for all the flow rates. MFIX will assign the correct sign to the computed velocity values.

If the mass or volumetric flow rate is specified for a mass outflow boundary condition, then at every interval BC_DT_0, MFIX will adjust the normal velocity so that the average computed-outflow rate is equal to the specified value. The user is cautioned, however, that if unrealistic mass flow rates are specified, the computations may become unstable. It is better to specify the

velocity at the mass outflow boundary, if some amount of fluctuation in the mass outflow rate is tolerable.

Keyword (dimension)	**Type**	**Description**
BC_VOLFLOW_g (bc)	DP	Gas volumetric flow rate through the boundary.
BC_VOLFLOW_s (bc, m)	DP	Solids volumetric flow rate through the boundary.
BC_MASSFLOW_g (bc)	DP	Gas mass flow rate through the boundary.
BC_MASSFLOW_s (bc, m)	DP	Solids mass flow rate through the boundary.

MFIX allows the specification of a transient jet with its velocity fluctuating between two values. The jet conditions will override the steady condition specified for the normal velocity. Therefore, if there is no transient jet, do not specify any of the following, except BC_DT_0, which may be required for mass outflow conditions.

Keyword (dimension)	Type	Description
BC_DT_0 (bc)	DP	The interval at the beginning when the normal velocity at the boundary is equal to BC_Jet_g0. When restarting, run this value and BC_Jet_g0 should be specified such that the transient jet continues correctly. MFIX does not store the jet conditions. For MASS_OUTFLOW boundary conditions, BC_DT_0 is the time period to average and print the outflow rates. The adjustment of velocities to get a specified mass or volumetric flow rate is based on the average outflow rate.
BC_Jet_g0	DP	Value of normal velocity during the initial interval BC_DT_0.
BC_DT_h (bc)	DP	The interval when normal velocity is equal to BC_Jet_gh.
BC_Jet_gh (bc)	DP	Value of normal velocity during the interval BC_DT_h.
BC_DT_1 (bc)	DP	The interval when normal velocity is equal to BC_Jet_g1.
BC_Jet_g1 (bc)	DP	Value of normal velocity during the interval BC_DT_1.

4.8 Internal Surfaces

Internal surfaces (IS) are normal to one of the coordinate directions and coincide with one of the faces of the scalar control volume. One of the three pairs of coordinates is equal. The surface is defined by the constant coordinates of each of the four edges, which can be specified with physical coordinates or cell indices, and the two equal values for the direction normal to the face, which can only be specified with physical coordinates. If cell sizes are not small enough to resolve a surface specified using physical coordinates, MFIX will indicate this problem with an error message.

To specify a large number of internal surfaces in a region, a 3D region may be specified. When IS_Type is specified for such regions, add a prefix (X_, Y_, or Z_) to indicate the direction of the internal surfaces; e.g., X_IMPERMEABLE specifies impermeable internal surfaces parallel to the X coordinate.

Internal surfaces act as free-slip walls in stress computations. This default condition cannot be changed.

Keyword (dimension)	Type	Description
IS_X_w (is)	DP	x coordinate of the west face or edge.
IS_X_e (is)	DP	x coordinate of the east face or edge.
IS_Y_s (is)	DP	y coordinate of the south face or edge
IS_Y_n (is)	DP	y coordinate of the north face or edge
IS_Z_b (is)	DP	z coordinate of the bottom face or edge
IS_Z_t (is)	DP	z coordinate of the top face or edge
IS_I_w (is)	I	i index of the west-most cell.
IS_I_e (is)	I	i index of the east-most cell
IS_J_s (is)	I	j index of the south-most cell
IS_J_n (is)	I	j index of the north-most cell
IS_K_b (is)	I	k index of the bottom-most cell
IS_K_t (is)	I	k index of the top-most cell
IS_TYPE (is)	C	Type of internal surface:
IMPERMEABLE or IP		No gas or solids flow through the surface.
SEMIPERMEABLE or SP		Only gas flows through the surface. Solids velocity is zero or a user-specified fixed value.
IS_PC (is, 2) (*, 1) = 1.E32 (*, 2) = 0.0	DP	1: permeability; 2: Inertial resistance coefficient. These values need to be specified for semipermeable surfaces only. The thickness used for pressure drop computation is that of the momentum cell (DX_e, DY_n, or DZ_t). To turn off the resistance, use a large value for permeability (1.E32) and a small value for the inertial resistance coefficient (0.0).
IS_VEL (is, m)	DP	Value of fixed solids velocity through semipermeable surfaces.

4.9 Output Control

Keyword (dimension)	Type	Description
RES_DT	DP	Interval at which restart (.RES) file is updated.
SPX_DT (9)	DP	Interval at which .SPX files are updated.
.SP1		Void fraction (EP_g).
.SP2		Gas pressure, solids pressure (P_g, P_star).

.SP3		Gas velocity (U_g, V_g, W_g).
.SP4		Solids velocity (U_s, V_s, W_s).
.SP5		Solids density (ROP_s).
.SP6		Gas and solids temperature (T_g, T_s1, T_s2).
.SP7		Gas and solids mass fractions (X_g, X-s).
.SP8		Granular temperature (G).
.SP9		User defined scalars.
OUT_DT	DP	Interval at which standard output (.OUT) file is updated.
USR_DT (5)	DP	Interval at which user-defined outputs are written from the subroutine WRITE_USR1.
NLOG [25]	I	Interval in number of time steps at which .LOG file is written.
FULL_LOG [.FALSE]	L	If true, display the residuals on the screen and messages about convergence on the screen and in the .LOG file.
RESID_STRING (8)	C	Specify resideuals to be printed as 4-character strings. First character specifies the field variable: P - pressure, R - density, U - u velocity, V - v velocity, W - w velocity, T - temperature, X _ species mass fraction, G - Granular temperature. The second number specifies the phase (0 for gas). The last two numbers specify the species index; e.g., 'P0' - gas pressure, 'R1' - solids phase 1 density, 'X001'- gas phase, species 1; 'X203' _ solids phase 2, species 3.

4.10 Chemical Reactions

Chemical reactions can be specified in two ways: in the data file, or in the subroutine rrates. If reactions are specified in the data file, MFIX uses the subroutine rrates0 to calculate all the required quantities. The user need not modify rrates0. If the chemical reactions are not specified in the data file, the user must program them into the subroutine rrates.

To define chemical reactions through the data file, first define species names with the following key word.

Keyword (dimension)	Type	Description
SPECIES_NAME	C	Names of gas and solids phase species. The first NMAX(0) are the names of gas species. The next NMAX(1) are the names of solids phase-1 species, and so on. All the names should be unique.

The reactions are specified in a reaction block beginning with the string @(RXNS) and ending with the string @(END). The reactions are entered in the following format: reaction name: reaction scheme. r1: CH4 + 2 O2 CO2 + 2H2O

The reaction rate in g-mol/(m^3.s)is then entered in the following format, starting with the keyword rate:

Keyword	**Name**	**Phase index for Temp** (m)	**Preexponen-tial Factor** (A)	**Tempera-ture Expo-nent** (n)	**Activation Temperature** (E/R)	**Concentrato n Dependence**
Rate	r1:	0	6.7E12	0	24358.	[O2]^1.3 [CH4]^0.2

The index m is used to identify the phase temperature to be used in the rate expression, to assign the enthalpy change caused by the reaction, and to determine the phase volume fraction to be used in the rate expression. m=0 is fluid phase, m=1 is solids phase 1, and so on. The rest of the input appears in the rate expression as follows:

rate = A * T_g**n * exp(-(E/R)/T_g)) * EP_g * (RO_g * X_O2/MW_O2)**1.3 * (RO_g * X_CH$/MW_CH4)**0.2

The rate expression may be written on multiple lines. Reverse reactions are denoted by a '<' in the reaction scheme.

The enthalpy change caused by the reaction in cal/g-mol is expressed as follows with the keyword DH. The default value is zero.

Enthalpy Change Keyword	**Reaction Name**	**Enthalpy Change Caused by Reaction** (cal/g-mol)
DH	r1:	-191759

The enthalpy change is assigned to the phase identified by the index m in the rate expression.

The following is an example of an athermal reversible reaction.

@(RXNS Start chemical reactions input)

A2R: A <--> R

rate A2R: 0 1.2E17 0 5837 [A]

rate A2R<: 0 2.5E41 0 14897 [R]

DH A2R: 0.0

@(END End chemical reactions input)

All the reaction schemes must be specified in the data file. All the reaction rate expressions and enthalpy changes need not be specified in the data file, however. If a rate expression or an enthalpy change is missing from the data file, that information must be added to the subroutine rrates0.

4.11 User-Defined Subroutines

The user may modify any *.f or *.inc file in MFIX. To modify a file, first copy it from the mfix/model directory into the run directory. Modify only this copy in the run directory; do **NOT** modify the original files in mfix/model. Then, invoke the 'sh make_mfix' command from the run directory. The make_mfix messages will identify the files from the run directory used to create the MFIX executable. All the (MFIX and non-MFIX) *.inc files from the run directory will be used to create the MFIX executable. Only MFIX *.f files from the run directory will be used, however. Non-MFIX *.f files in the run directory will be ignored. To use new Fortran files, include them in one of the MFIX *.f files.

The following is a list of MFIX files that are usually modified to include chemical reactions and user defined scalars:

rrates.f	Chemical reation rates and heats of reaction.
transport_prop.f	Transport properties.
physical_prop.f	Physical properties.
scalar_prop.f	Properties and source terms in scalar transport equations.

The following routines are used for writing user-defined output:

write_usr0.f	Called once during the run. Can be used for opening user-defined files.
write_usr1.f	Called at intervals defined by USR_DT.

To activate the calls to the following three routines, set call_usr = .TRUE. in the data file:

usr0.f	A subroutine that is called once every run, just before the time-loop begins.
usr1.f	A subroutine that is called once every timestep.

usr2.f	A subroutine that is called once every iteration.
usr3.f	A subroutine that is called once every run, after the time-loop ends.
usrnlst.inc	List of user-defined keywords. These may be used to enter data through the input data file mfix.dat.
usr_init_namelist.f	Initialize user-defined keywords.
usr_mod.f	User-defined module. Include "Use usr" to use user-defined variables in this module. If allocatable arrays are defined in this module, allocate them in usr0.f.

4.12 Parallelization Controls

Keyword (dimension)	Type	Description
NODESI [1]	I	Number of grid blocks in x-direction.
NODESJ [1]	I	Number of grid blocks in y-direction.
NODESK [1]	I	Number of grid blocks in z-direction.

NODESI * NODESJ * NODESK must be the same as the number of processors specified using the mpirun (or equivalent command). Otherwise the code will return with an error.