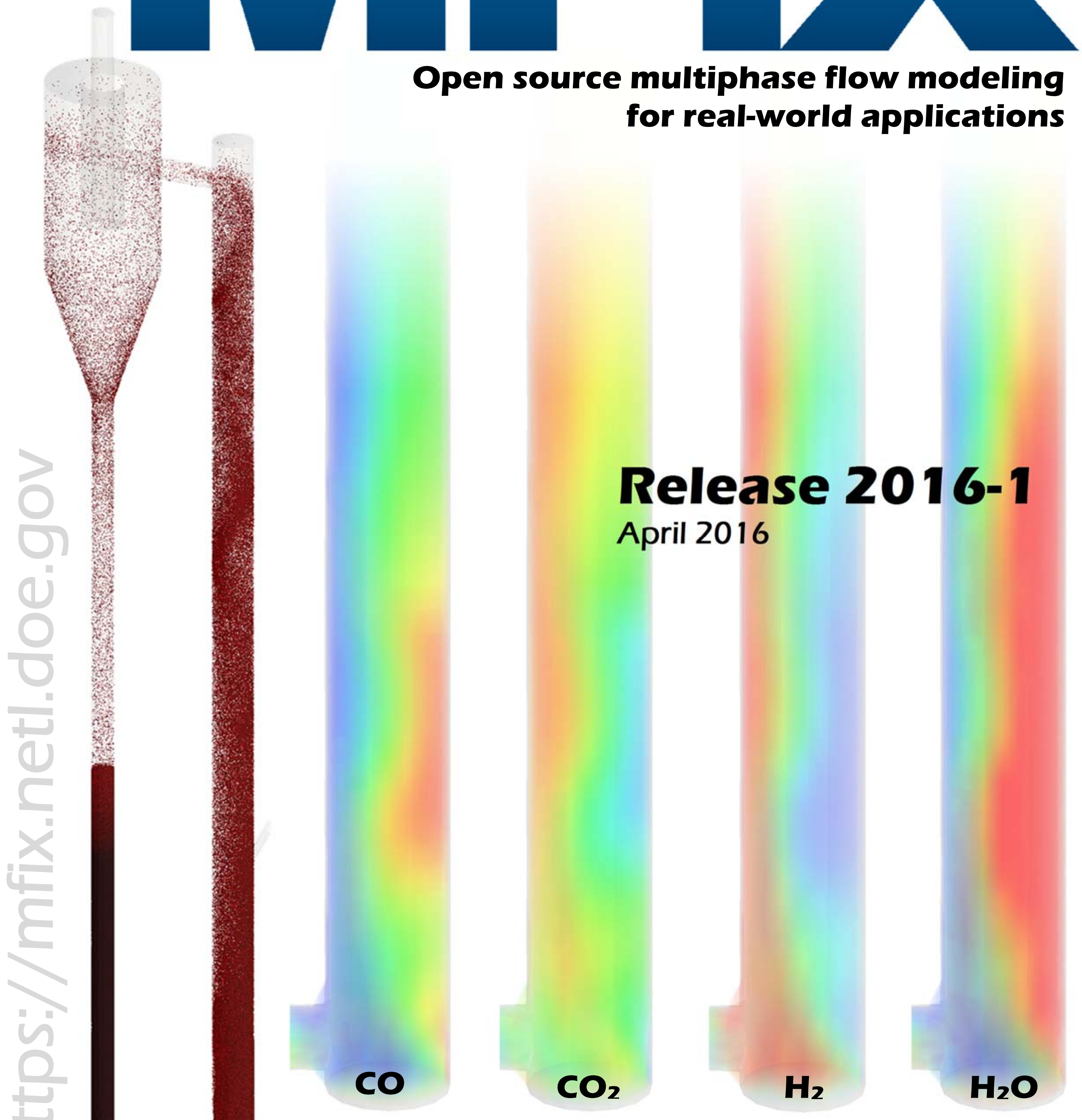
MFiX

Open source multiphase flow modeling for real-world applications

Release 2016-1

April 2016

https://mfix.netl.doe.gov



MFIX-DEM simulation of a reacting circulating fluidized bed with over 10^7 particles. (Left) The full-loop geometry with particles colored by temperature. (Right) Inlet region volume rendering of gas phase mass fractions.

NETL

Image credits:

Cover page: Jordan Musser, DOE NETL: MFIX-DEM simulation of a chemically reacting circulating fluidized bed with over 10^7 particles.

Page 8, top: Aytekin Gel, *ALPEMI Consulting, LLC*: MFIX-TFM simulation of coal jet penetration, colored by CO2 species mass fraction.

Page 8, bottom: Jordan Musser, *DOE NETL*: Reactive MFIX-DEM simulation of a spouted bed, particles colored by temperature.

Page 9, top: Rahul Garg, *URS E&C Inc.*: MFIX-PIC simulation of a cyclone, showing particles and streamlines, colored by velocity.

Page 9, bottom: Jordan Musser, *DOE NETL*: MFIX-Hybrid simulation of a bubbling bed with two solids phases (one continuous phase and one discrete phase). The background is colored by solids bulk density (continuous phase) and spheres represent the second solids phase.

Notice

Disclaimer

Table of Contents

1 Introduction

MFIX is an open-source multiphase flow solver and is free to download and use. A one-time no-cost registration is required prior to downloading the source code. To register, go to https://mfix.netl.doe.gov/ and click on the "Register" button in the upper right corner. Once you have read the notice, you can submit your application by clicking on "REGISTER." After your application has been reviewed and accepted, you will receive an email notification and instructions on how to download the code. Please allow for 2-3 business days for your registration to be processed.

Potential users may find reviewing the Frequently Asked Questions section of the MFIX website useful before downloading the code.

The MFIX distribution contains the following:

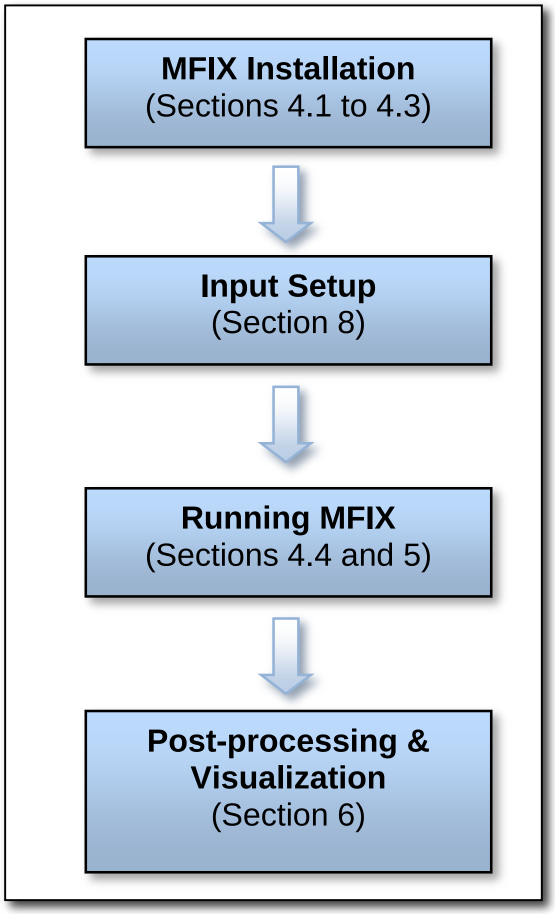
Item	**Description**
model	Source files for MFIX, the multiphase flow solver.
post_mfix	Source files for POSTMFIX, a text-based program to process MFIX simulation data.
tutorials	Example problems, some containing documentation describing the simulation setup which new users may find useful.
tests	Test simulations used to verify the code during development.
tools	Various utilities and development tools.
doc	MFIX documentation (in pdf format)
benchmarks	Test cases used to collect timing and profiling data.

In addition to POSTMFIX, the open-source tools ParaView and VisIt can also be used to both visualize and post-process MFIX results. They are available at:

ParaView:	http://www.paraview.org/
VisIt:	https://wci.llnl.gov/codes/visit/home.html

Please follow the instructions on the above websites to install ParaView or VisIt.

The following chart provides a workflow overview with related sections in this document for quick review.

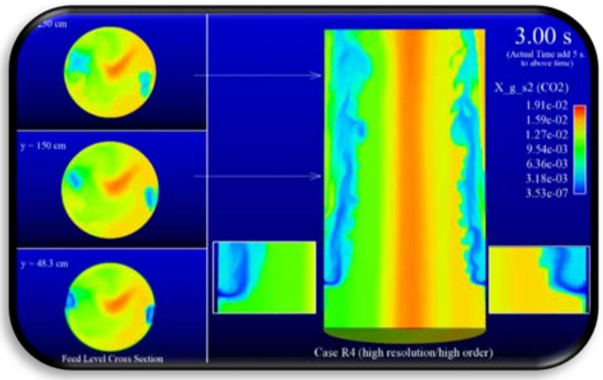


2 Development state of MFIX models

MFIX provides a suite of models that treat the carrier phase (typically the gas phase) and disperse phase (typically the solids phase) differently. Their current state of development is summarized in the tables below.

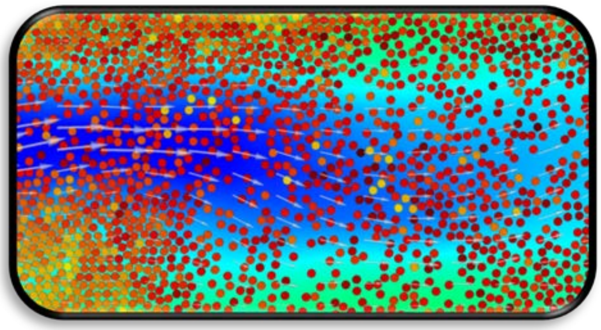
MFIX-TFM (Two-Fluid Model) is an Eulerian-Eulerian model, which supports a broad range of capabilities for dense, reacting, multiphase flows by representing the fluid and solids as interpenetrating continua. This is the most mature MFIX model and is capable of modeling multiphase reactors ranging in size from benchtop to industry-scale. Approximation of the solid phase as a continuum typically allows for faster simulation time than Lagrangian techniques; however, it also introduces the need for accurate mathematical models to capture realistic solids phase behavior. This includes transport properties, heterogeneous reaction kinetics, and constitutive relations for interaction between fluid and solid phases, e.g., solids phase drag and interphase heat transfer.

	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●	●	●
Species Equations	●	●	●
Chemical Reactions	●	●	
Cartesian cut-cell	●	●	□



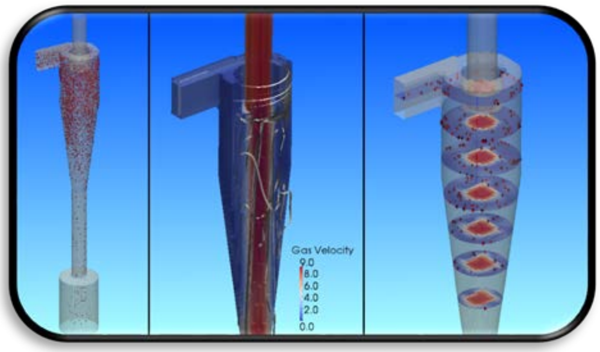
MFIX-DEM (Discrete Element Model) is an Eulerian-Lagrangian model that treats the fluid phase as a continuum and models the individual particles of the solid phase. This is a relatively new variation on MFIX. While the treatment of individual particles can provide higher fidelity over a broad range of flow regimes (from dilute to packed), it also very challenging when dealing with very large numbers of particles for large-scale simulations. These large-scale applications will require high performance computing (HPC) resources and large amounts of computer time. Code optimization and speed up are critical research fronts to support industrial scale applications.

	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●	●	
Species Equations	●	●	
Chemical Reactions	●	●	
Cartesian cut-cell	○	○	



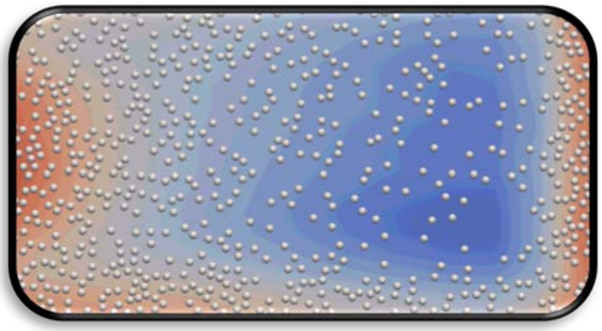
MFIX-PIC (Multiphase Particle in Cell) is another Eulerian-Lagrangian model that represents the fluid as a continuum while using "parcels" to represent groups of real particles with similar physical characteristics. The MFIX-PIC approach offers reduced computational cost over MFIX-DEM as there are typically few parcels to track and parcel collisions are not resolved. However, the added modeling approximations influence the overall accuracy of the method. Development, validation, and optimization of modeling approximations are critical research fronts.

	Serial	[†]DMP	[‡]SMP
Momentum Equations	●		○
Energy Equations			
Species Equations			
Chemical Reactions			
Cartesian cut-cell	○		□



MFIX-Hybrid (Eulerian-Lagrangian-Eulerian) is a blend of MFIX-TFM and MFIX-DEM that represents the fluid as a continuum and models solids as either a continuous phase (TFM) or discrete particles (DEM). This technique is presently restricted to solving only the momentum equations to yield hydrodynamic predictions. This model is still in its infancy and has seen only limited testing.

	Serial	[†]DMP	[‡]SMP
Momentum Equations	○	○	○
Energy Equations			
Species Equations			
Chemical Reactions			
Cartesian cut-cell	○	○	○



● – implemented and fully tested
○ – implemented with limited testing
□ – not tested or status unknown

† Models not extended to DMP-parallel are only available for serial runs.
‡ Models not extended to SMP-parallel are available for SMP runs but do not scale with thread count.

3 Release notes for 2016-1

For MFIX users upgrading to the 2016-1 Release, please note the following changes from the previous (2015-2) release:

Backward compatibility is not ensured for either input or restart files. Please contact the development team through the mailing list if you have difficulties running a previous model with the new release.

New features:

- **DMP support for DEM thermochemistry** – MFIX-DEM simulations with heat transfer and/or chemical reactions now support parallel execution. This allows for larger particle counts in reacting flow simulations with reduced time-to-solution for greater modeling capability of MFIX-DEM.
- **DEM particle-wall heat transfer** – MFIX-DEM particles may exchange heat with the domain boundaries via specified constant wall temperature boundary conditions. The rotating drum with particle-wall heat transfer tutorial illustrates this new feature (tutorials/DEM_Wall_HT).

Improved Features:

- **Greater UDF capabilities** – Users may construct user-defined functions (UDFs) to specify source terms to the governing equations and many transport coefficients and field properties. This allows for faster model development by removing the need to modify master source routines. See usr_source.f and usr_prop.f routines and the UDF keyword section for more information.

4 MFIX on a UNIX/LINUX Workstation

MFIX is primarily designed to run on Linux operating systems and this section describes the preferred way of building and running MFIX.

Users should be familiar with basic Linux operating system commands and procedures before attempting to build and run MFIX.

Carefully read and follow these instructions. Check the mailing list archives if you have problems building or running MFIX as your question may have been answered previously. Information on the mailing lists is provided at the end of this document.

4.1 Prerequisites

To build MFIX, the following must be installed on your system. Contact your system administrator for assistance if necessary.

- **Fortran compiler**. Commonly available compilers include:
    - GCC (gfortran) version 4.3 and above
    - Intel (ifort) version 11.1 and above

- **GNU Autoconf** version 2.69 or greater is required when building from source code obtained from the MFIX git repository. This does not apply to the source code tarball on the MFIX website.

4.2 Extracting the MFIX directory

MFIX is distributed as a compressed source tar ball named **mfix-2016.1.tar.gz**. To decompress and extract the tar file:

```
> tar xzf mfix-2016.1.tar.gz
```

Here it is assumed that you are in the directory containing the tar ball. Extracting the tar ball creates a directory named **mfix-2016.1** containing the MFIX and POSTMFIX source codes, tests and tutorials, as well as some additional documentation and utilities.

4.3 Building MFIX

MFIX is built using GNU Autoconf, which is a general tool for producing configure scripts for building and installing software on different computer systems. First, run the shell script **configure_mfix** to create a Makefile, then run GNU Make to build the MFIX executable. A step-by-step tutorial is presented at the end of this section.

4.3.1 Configuring with configure_mfix

This section focuses on the **configure_mfix** script and the availability of several flags. **configure_mfix** is a wrapper for the usual GNU Autoconf configure script.

Alias creation (optional)

For convenience, an alias can be created to avoid specifying the path to the MFIX configure script. Assuming the MFIX source was extracted in the home directory, and you are using the C shell, an alias can be created by executing:

```
> echo "alias configure_mfix ~/mfix-2016.1/configure_mfix" >>
~/.cshrc
```

This appends the quoted text to the .cshrc file located in the home directory. The alias will take effect the on the next login or after sourcing the .cshrc file. To source the .cshrc file in the current terminal, enter at the prompt:

```
> source ~/.cshrc
```

Afterwards, MFIX can be configured from any directory by running the alias, **configure_mfix**. Users familiar with the creation of aliases may choose other various ways to define an alias (e.g., directly editing the .cshrc or .cshrc_aliases files). Users that use a different shell should create an alias with the respective shell resource file (e.g. bash shell users ~/.bashrc).

Passing arguments to the build script

Arguments may be passed to the build script to specify various options: compiler, optimization flags, SMP/DMP support, and other options. All configuration options can be displayed with:

```
> ~/mfix-2016.1/configure_mfix --help
```

The most common arguments are given in the following table.

Argument	Description
FC=*NAME*	Specify the Fortran compiler command
F77=*NAME*	Specify the Fortran 77 compiler command
FCFLAGS='*FLAGS*'	Specify compiler flags
--dmp	Enable distributed memory support (MPI)
--smp	Enable shared memory parallel support (OpenMP)

It is recommended to ***always*** specify the desired compiler and flags to avoid unwanted compiler selection and default build options.

Specifying the Fortran compiler (optional but recommended)

The Fortran compiler is specified by passing the **FC** argument to **configure_mfix**. If the **FC** argument is not specified, the script will search the environment for a Fortran compiler (usually gfortran). The **configure_mfix** script will test the Fortran compiler with any specified flags (covered next). If the compiler is not found or if the compiler gives an error, the Makefile will not be generated and detailed error messages will be in config.log. When seeking help on the mailing list for build issues, include the config.log file for assistance.

The Fortran 77 compiler is specified by the **F77** argument to the **configure_mfix** script. By default, F77 is set to the same compiler specified by the FC argument. However, on some systems F77 may need to be defined separately.

Common compilers are given in the following table.

Compiler	Description
gfortran	GNU Fortran compiler (serial/smp)
ifort	Intel Fortran compiler (serial/smp)
mpif90	Generic MPI Fortran wrapper (dmp/combined smp-dmp)
mpifort	Generic MPI Fortran wrapper (dmp/combined smp-dmp)
mpiifort	Intel MPI Fortran wrapper (dmp/combined smp-dmp). *Older versions commonly use the mpif90 command.*

Specifying compiler options (optional)

Compiler flags are specified by passing the **FCFLAGS** argument to **configure_mfix**. If the **FCFLAGS** argument is not specified, the compiler defaults are used in building the executable. The **configure_mfix** script will test the compiler with the specified flags. If the compiler is not found or if the compiler gives an error with the given flags, the Makefile will not be generated and detailed error messages will be in config.log. When seeking help on the mailing list for build issues, include the config.log file for assistance.

Each compiler has different default behavior. Consult the compiler's manual for a complete listing of available options.

Common compiler flags for **GNU Fortran** are given in the following table.

GNU Fortran	Option	Description
	-g	Produce debugging information
	-O0, -O1, -O2, -O3	Optimization level (refer to the compiler manual for specific information about each optimization level). Typically, the following are used: -O0 *debugging* -O2 *production executables*
	-fcheck=all	Generates runtime checks useful for debugging.
	-fbacktrace	Proved a full backtrace when a runtime error is encountered for debugging.

Common compiler flags for **Intel Fortran** are given in the following table.

Intel Fortran	Option	Description
	-g	Produce debugging information
	-O0, -O1, -O2, -O3	Optimization level (refer to the compiler manual for specific information about each optimization level). Typically, the following are used: -O0 *debugging* -O2 *production executables*
	-check all	Generates runtime checks useful for debugging.
	-debug	Generates complete debugging information

4.3.2 Building mfix with GNU make

If the configure script successfully created a Makefile (see above), then the next step is to build MFIX by running GNU make command.

```
> make
```

The -j option may be used build in parallel which may decrease compile time.

```
> make -j
```

Note that on some systems parallel builds may fail due to file dependencies (e.g., file1 depends of file2 which has not been compiled yet). Typically, running the **make** command again will overcome these errors. If compiling and linking are successful, an executable named **mfix** along with a few intermediate build files will be in the current directory.

The generated executable is **mfix** which differs from previous releases in which the executable was **mfix.exe**. In the current release, the executable is only named mfix.exe on Windows (see section 9.2).

4.3.3 Building MFIX: A step-by-step tutorial

The following example shows how to build and run the **fluidbed1** tutorial. This example assumes you have the GNU Fortran compiler (gfortran) installed.

To begin, go to the fluidbed1 tutorial directory and list its contents:

```
> cd ~/mfix-2016.1/tutorials/fluidbed1
> ls
```

```
mfix.dat
```

As shown this folder contains the input file, **mfix.dat**, which specifies the simulation setup. This file is only needed to compile MFIX when user-defined reaction files are present (e.g., **usr_rates.f**). However, the mfix.dat file must be present when running MFIX, the last step of this tutorial.

The directory where MFIX will be run is called the run directory (RUNDIR). Here the run directory is **fluidbed1**, and it currently contains only the mfix.dat file.

Running the **configure_mfix** script and specifying the compiler and optimization flags:

```
> ../../configure_mfix FC=gfortran FCFLAGS='-g -O2'
```

The above commands runs **configure_mfix** by specifying the relative path (two levels up). Alternatively, we could specify the absolute path:

```
> ~/mfix-2016.1/configure_mfix FC=gfortran FCFLAGS='-g -O2'
```

or use the alias created in section 4.3.1:

```
> configure_mfix FC=gfortran FCFLAGS='-g -O2'
```

If the configure script successfully created a Makefile, build MFIX by running make.

```
> make
```

The build may take several minutes to complete. If the build is successful, the executable will be in the run directory.

```
> ls
mfix.dat    mfix
```

Finally, the simulation is started by entering:

```
> ./mfix
```

For details see the next section.

4.4 Running MFIX

This section provides basic guidance for running MFIX in serial, SMP, and DMP modes. Contact your system administrator about the policies and procedures for running on your system as you may be required to submit jobs through a queuing system.
MFIX requires an mfix.dat file in the run directory (RUNDIR). For instance, to run the fluidbed1 tutorial:

```
> cd ~/mfix-2016.1/tutorials/fluidbed1
> ls
mfix.dat     mfix
```

For your own simulation, you can start with one of the predefined mfix.dat files and customize it. See Section 7 for a full list of keyword options available in mfix.dat.

4.4.1 Serial Execution

MFIX can be launched in different ways in order to manage screen output. The simplest way is to directly run the executable:

```
> ./mfix
```

This approach runs MFIX in the foreground and output messages from MFIX are sent to the terminal.
If you want to run your MFIX job in the background, redirect MFIX output to a log file:

```
> ./mfix >& run.log &
```

You can check the progress of your job by printing the log file to your terminal:

```
> tail -f run.log
```

To stop the tail command type Ctrl+C at any time. This will not interrupt your job.

4.4.2 SMP Execution

Shared memory parallel (SMP) utilizing OpenMP directives, is enabled by passing the SMP flag to the build script.

```
> configure_mfix --smp FC=gfortran FCFLAGS='-g -O2' && make
```

The number of threads are set at runtime through the environment variable OMP_NUM_THREADS. For example, four threads can be used during a simulation in a bash shell session by entering:

```
> export OMP_NUM_THREADS=4
```

The same environment variable can be set in csh by entering:

```
> set OMP_NUM_THREADS 4
```

After the OMP_NUM_THREADS variable is specified, an SMP job is launched in the same manner as a serial run. For example, to run your SMP MFIX job in the background and redirect messages to a log file:

```
> ./mfix >& run.log &
```

4.4.3 DMP Execution

Distributed memory parallel (DMP) support through Message Passing Interface (MPI) is enabled by passing the DMP flag to the build script:

```
> configure_mfix --dmp FC=mpif90 FCFLAGS='-g -O2' && make
```

Your MPI compiler wrapper may be mpif90, mpifort, or mpiifort depending on your system, your compiler, and your MPI implementation.
The number of MPI ranks is specified at runtime. The actual command to run the job is specific to the compiler and MPI library on your system. For example, an MFIX executable built with the GNU Fortran compiler and OpenMPI libraries might be launched with four MPI processes and run in the background with standard I/O messages redirected to a log file by entering:

```
> mpirun -np 4 ./mfix >& run.log &
```

Again, the actual command can vary from system-to-system.

Verify that your MPI installation works properly if you intend to compile and run the DMP version of MFIX. Contact your system administrator if you are not sure how to proceed.
(see mfix-2016.1/tools/mpi/ MPI_verification_for_MFIX.pdf)

4.5 Building POSTMFIX

Before building POSTMFIX, verify that there is a working Fortran compiler on your system. Contact your system administrator if you have questions regarding the availability of Fortran compilers.

After building MFIX, you can build postmfix in the run directory:

```
> cd ~/mfix-2016.1/tutorials/fluidbed1
> make postmfix
```

The build may take several minutes to complete. Upon successful compilation, the executable is copied into the current directory.

```
> ls
mfix.dat     mfix     postmfix
```

Once built, postmfix may be used to extract data from a particular location in the domain or perform some basic averaging of flow field data.

4.6 Enabling NetCDF Output

NetCDF is an open standard format for scientific data that may perform better than RES files for some large simulations. Unlike the other output formats, NetCDF support requires an external library to be linked with MFIX at build and runtime. To build MFIX with NetCDF support, first set the environment variables for the NetCDF include directory, `NETCDF_INCLUDE`, and the NetCDF library, `NETCDF_LIB`:

```
> export NETCDFF_INCDIR=/path/to/netcdf/include/directory
> export NETCDFF_LIBDIR=/path/to/netcdf/lib/directory
```

Contact your system administrator for information regarding the availability and usage of NetCDF.

If NetCDF is installed on your system and available in your environment path, you may be able to locate the *include* and *lib* directories by using the nf-config utility. To determine if the installation includes the Fortran 90 API:

```
> nf-config --has-f90
```

Contact your system administrator if your installation does not include the Fortran 90 API. The location of the *include* and *lib* directories is obtained with the following commands:

```
> nf-config --includedir
> nf-config --flibs
```

These commands may return additional linking information that is not needed to build MFIX with NetCDF support. Only the paths to the *include* and *lib* directories need to be specified for the MFIX build script.

Next, specify the flag to enable NetCDF support when launching the MFIX build script:

```
> configure_mfix --enable-netcdf [... usual options ...]
> make
```

At runtime, it may be necessary to set `LD_LIBRARY_PATH` to include NetCDF if it is not installed in a standard location.

```
> export LD_LIBRARY_PATH=/path/to/netcdf/lib/directory
> ./mfix
```

Again, contact your system administrator for information on how to use external libraries such as NetCDF.

Use the keyword `BWRITE_NETCDF` to enable NetCDF output (See section 8.11). MFIX generates NetCDF output files as <RUN_NAME>_###.nc, which can be loaded into ParaView.

5 MFIX at Run Time

5.1 MFIX Output and Messages

MFIX generates several output files during a simulation. The following table provides an overview of these files and their purpose.

Extension	Type	Description
.LOG	ASCII	Contains messages about the run. Processor specific log files may be generated for DMP runs.
.OUT	ASCII	Echoes the input file and shows the numerical cell distribution. Field variables are also written if OUT_DT is defined in the mfix.dat file.
.RES	Binary	Double precision file used for restarts.
.SPx	Binary	Multiple singe precision files used to store transient simulation data for post processing.

If the data file specifies FULL_LOG = .TRUE., then the progress of the run is displayed in the terminal as shown below. The normalized residuals for various equations are written out for each iteration and every time-step.

```
Time = 0.92965    Dt = 0.13930E-02
 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 simulation time and current time-step. 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 specified with the keyword RESID_STRING.

MFIX uses a variable time step to reduce run time by automatically adjusting the step size within user-defined limits. As a result iterations may not converge at larger time-step sizes. When this happens, the time step size is reduced successively until convergence is obtained. Messages about divergence and recovery are recorded in the .LOG file and displayed in the terminal if FULL_LOG = .TRUE..

MFIX reports errors while reading and processing the mfix.dat file, and during a run. Errors in reading the data file and in opening files are reported to the terminal. All other errors are written to the.LOG. Additionally, runtime errors are displayed to the terminal if

FULL_LOG=.TRUE..

While reporting errors in reading the data file, MFIX displays the problematic line of input, so that the error can be easily detected. Possible causes of error are (1) incorrect format for the name-list input, (2) unknown (possibly misspelled) keyword, 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 number of time steps, MFIX checks whether that

- mass fractions sum to 1.0
- overall interphase mass transfer sums to zero
- viscosities, conductivities, and specific heats are nonnegative
- temperatures are within specified bounds

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 steps, 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.

5.2 Restarting a Run

A stopped run can be restarted by launching MFIX after specifying RUN_TYPE = 'restart_1' in mfix.dat. The old .OUT file will be overwritten and new messages are appended to the existing .LOG file.

5.3 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. 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), convergence may 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.

6 Post Processing and Visualization

MFIX can generate output data in several formats for visualization and analysis. The command line tool POSTMFIX is distributed with MFIX. In addition the open source GUI tools ParaView (www.paraview.org version 4.1 or later recommended) and VisIt (https://wci.llnl.gov/simulation/computer-codes/visit/) support some of the MFIX output file formats.

Filename	File Type	Fluid data?	Particle data?	Process with POSTMFIX?	Open in ParaView?	Open in VisIt?
<RUN_NAME.RES	MFIX Binary	Yes	No	Yes	Yes	Yes
<RUN_NAME>_###_DES.RES	MFIX Binary	No	Yes	No	No	No
<RUN_NAME>_###.nc	NetCDF	Yes	No	No	Yes	Yes
<RUN_NAME>.pvd	VTK	Yes	No	No	Yes	No
<RUN_NAME>_###.vtu	VTK	Yes	No	No	Yes	Yes
<VTK_REGION>.pvd	VTK	Yes	No	No	Yes	No
<VTK_REGION>_###.vtu	VTK	Yes	No	No	Yes	Yes
<RUN_NAME>_DES.pvd	VTK	No	Yes	No	Yes	No
<RUN_NAME>_DES_###.vtp	VTK	No	Yes	No	Yes	Yes
<VTK_REGION>.pvd	VTK	No	Yes	No	Yes	No
<VTK_REGION>_###.vtp	VTK	No	Yes	No	Yes	Yes

Notes:

1. *pvd files only contain information linking the respective .vtu and .vtp files to time-step information.*
2. <VTK_REGION>_###.vtp *files are binary files. The* <RUN_NAME>_DES_###.vtp are ASCII files.

6.1 Running POSTMFIX

The POSTMFIX tool is used for reading the binary MFIX .SPx output files and outputting data in text files. The following walk through demonstrates how to run POSTMFIX on the results from the FluidBed_DES tutorial with the default settings. The postmfix executable is assumed to be built or copied into the run directory.
After launching the executable, enter the run name.

```
> ./postmfix
Enter the RUN_NAME to post_process > DES_FB1    ← DES_FB1<Enter>
```

A simple menu of options is presented. Type ‘1’ to examine/print data and press Enter.

```
 *************************************************
  0   - Exit POST_MFIX
  1   - Examine/print data
  2   - Write .RES from data in .SPx files
  3   - Write .RES for a new grid, using old data
  4   - Calculate miscellaneous quantities
  5   - Print out variables
  6   - Call user defined subroutine USR_POST
  7   - Write a new SPx file with selected records
  8   - Write new SPx files with time averaged data
  9   - Perform ORNL calculations
 10   - run scavenger code
 *************************************************
Enter menu selection > 1

 Interactive data retrieval program. Type ? any time for help,
 or press RETURN to select default values shown in parenthesis.
```

Type F to use the default data precision and press Enter.

```
Write output using user-supplied precision? (T/F) F ← F<Enter>
```

Enter a time range for data extraction and analysis. The default simulation has a simulation length of one second, so enter a range from 0.1 seconds to 0.9 seconds. The next prompt asks if the data should be time averaged. Press Enter to skip the averaging.

```
Time: (  0.000,  0.000) > 0.1, 0.9
Time average ? (N) >          ←     <Enter>
```

Enter the variable of interest. The default is the gas phase volume fraction, EP_G. A complete list of possible entries is given by typing ‘?’ and Enter. Press Enter to select the gas phase volume fraction.

```
Variable: (EP_g     ) >       ←     <Enter>
```

Next enter the spatial range to extract the data. This requires an understanding of the I/J/K values for your simulation. Basic geometric information for the simulation is provided in the .OUT file. For this example, we will take a vertical slice from the approximate center of the 2D domain.

```
I range: (  1,  1) >8,8       ←     8,8<Enter>
J range: (  1,  1) >2,40      ←     2,40<Enter>
Average or sum over J? (N) >  ←     <Enter>
K range: (  1,  1) >          ←     <Enter>
```

Specify where to output the data. Press Enter to select the default *, printing the data to the terminal. Alternatively, specify a file name to save the data.

```
File: (*           ) >   ←  <Enter> prints to screen
                           (filename<Enter> saves to filename)
 X =   6.5000
 Z = -0.20000
 Time =  0.10075
     Y              EP_g
     1.0000    0.43971
     3.0000    0.45994
        ....etc....
```

Return to the original time prompt to continue data extraction or analysis. Type ‘q’ and Enter to return to the main menu. From the main menu, type ‘0’ and Enter to exit.

```
Time: (  1.000,  1.000) > q      ←    q<Enter> to quit

< main menu is displayed again >

Enter menu selection > 0        ←    0<Enter> to exit
```

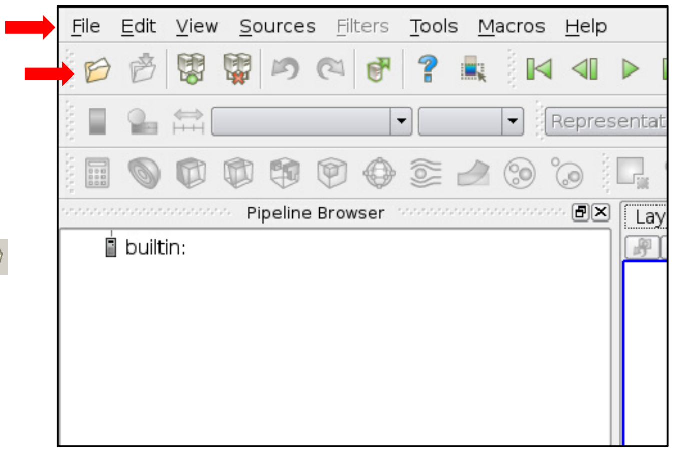
6.2 ParaView

This walk through demonstrates how to use ParaView to visualize the results of the FluidBed_DES tutorial. It is assumed that the FluidBed_DES tutorial was successfully run with default settings and that ParaView is installed on your system. First the tutorial demonstrates how to visualize the fluid field; then the DEM particles are added using spherical glyphs.

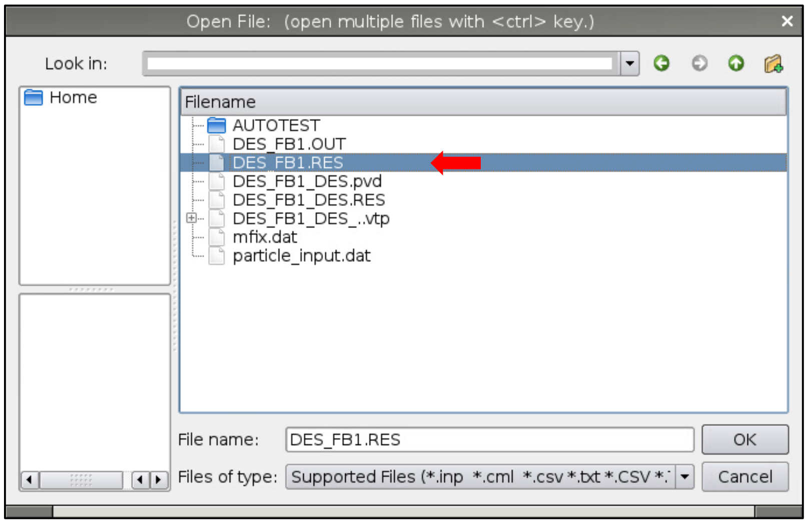
Fluid field results for a standard structured mesh are displayed in ParaView by loading the .RES file. To open the files select

File > Open
Similarly, you can click on the icon

Once the file is loaded, you need to click on the green "Apply" button to load all of the variables.

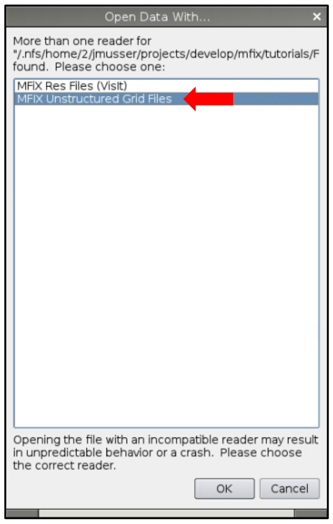


When prompted, select the **DES_FB1.RES** file. **Do not load the DES restart file (DES_FB1_DES.RES)**. This binary file is not supported by any visualization software. It only contains restart data and will likely cause ParaView to crash if loaded.



AUTOTEST
DES_FB1.OUT
DES_FB1.RES
DES_FB1_DES.pvd
DES_FB1_DES.RES
DES_FB1_DES_..vtp
mfix.dat
particle_input.dat

File name: DES_FB1.RES
Files of type: Supported Files (*.inp *.cml *.csv *.txt *.CSV *.



More than one reader for "/.nfs/home/2/jmusser/projects/develop/mfix/tutorials/F found. Please choose one:

MFIX Res Files (VisIt)
MFIX Unstructured Grid Files

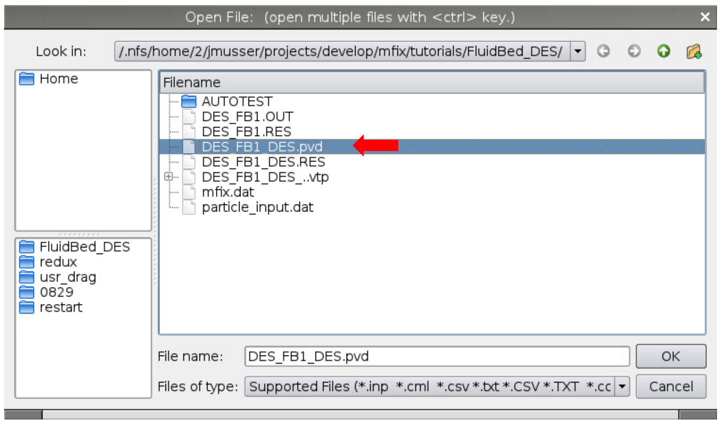
Opening the file with an incompatible reader may result in unpredictable behavior or a crash. Please choose the correct reader.

Newer versions of ParaView require that you select the appropriate reader. Choose to open the data with the 'MFIX Unstructured Grid Files'.

ParaView typically displays the gas phase volume fraction once the data is loaded. It may be necessary to rescale the data range as the initial range may only be suitable for displaying the initial conditions. This can be done by clicking the button.

DEM and PIC particle simulation data is loaded into ParaView by opening the **.pvd** file.

Again, click on the green "Apply" button to load all of the variables.



Look in: /.nfs/home/2/jmusser/projects/develop/mfix/tutorials/FluidBed_DES/

FluidBed_DES
redux
usr_drag
0829
restart

AUTOTEST
DES_FB1.OUT
DES_FB1.RES
DES_FB1_DES.pvd
DES_FB1_DES.RES
DES_FB1_DES_..vtp
mfix.dat
particle_input.dat

File name: DES_FB1_DES.pvd
Files of type: Supported Files (*.inp *.cml *.csv *.txt *.CSV *.TXT *.cc

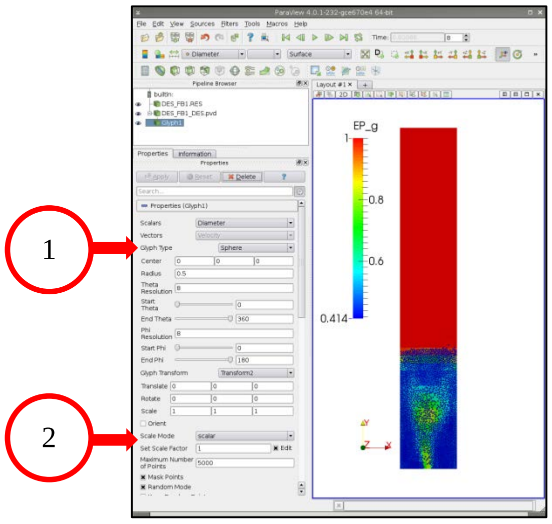
Particles are shown by applying a glyph to the dataset. To apply a glyph filter:

Filters > Alphabetical > Glyph

Similarly you can click the icon:

Commonly, particle data is represented using:

1. ‘Sphere’ glyph type and
2. Scalar scale mode with a scale factor of one.



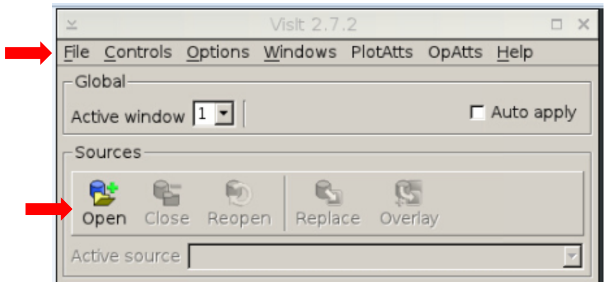
Scalars: Diameter
Vectors: Velocity
Glyph Type: Sphere
Center: 0 0 0
Radius: 0.5
Theta Resolution: 8
Start Theta: 0
End Theta: 360
Phi Resolution: 8
Start Phi: 0
End Phi: 180
Glyph Transform: Transform2
Translate: 0 0 0
Rotate: 0 0 0
Scale: 1 1 1
Orient: ☐
Scale Mode: scalar
Set Scale Factor: 1 ☒ Edit
Maximum Number of Points: 5000
☒ Mask Points
☒ Random Mode

Note that these screenshots may appear differently depending on your version of ParaView.

6.3 VisIt

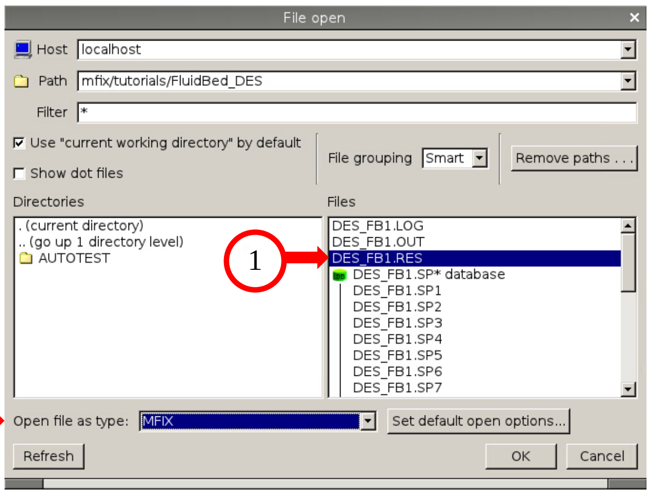
This walk through demonstrates how to use VisIt to visualize the results of the FluidBed_DES tutorial. It is assumed that the FluidBed_DES tutorial was successfully run with default settings and that VisIt is installed on your system. First the tutorial demonstrates how to visualize the fluid field; then the DEM particles are added using spherical glyphs. The screen shots and menu structure were taken from VisIt version 2.7.2 and may be different in different versions.

Fluid field results for a standard structured mesh are displayed in VisIt by loading the .RES file.
To open the files select
File > Open
Similarly, you can click on the ‘Open’ icon.

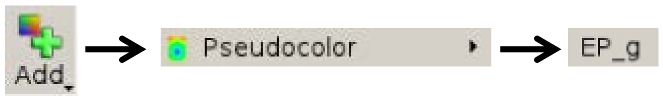


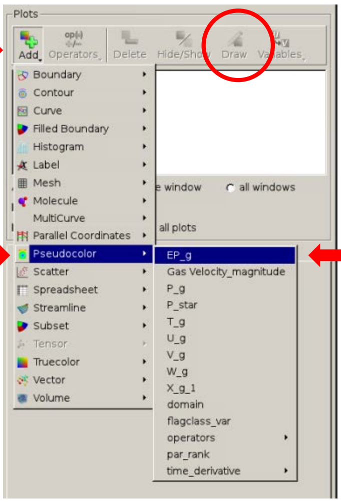
In the ‘File Open’ dialog:
(1) Select the **DES_FB1.RES** file. **Do not load the DES restart file (DES_FB1_DES.RES)**. This binary file is not supported by any visualization software. It only contains restart data and will likely cause VisIt to crash if loaded.

(2) Specify the ‘Open file as type’ as MFIX. Failing to select MFIX as the file type typically results in an error.


File open
Host: localhost
Path: mfix/tutorials/FluidBed_DES
Filter: *
[✓] Use "current working directory" by default
[ ] Show dot files
File grouping: Smart
Directories:
. (current directory)
.. (go up 1 directory level)
AUTOTEST
Files:
DES_FB1.LOG
DES_FB1.OUT
DES_FB1.RES
DES_FB1.SP* database
DES_FB1.SP1
DES_FB1.SP2
DES_FB1.SP3
DES_FB1.SP4
DES_FB1.SP5
DES_FB1.SP6
DES_FB1.SP7
Open file as type: MFIX

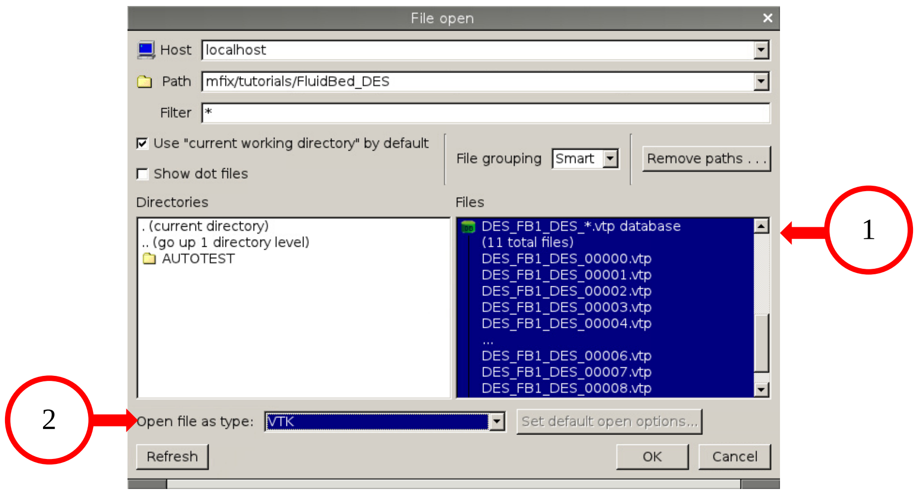
The gas phase volume fraction is plotted by

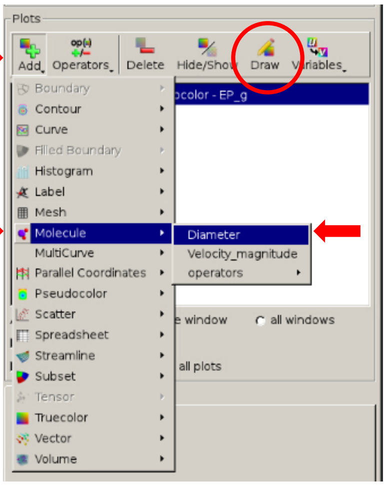




Once a field variable is selected, it is displayed by clicking the Draw button. This button is unavailable until an item is selected from the Plots menu.

DEM and PIC particle simulation data is loaded into VisIt by opening the (1) ***.vtp database**. (2) Specify the ‘Open file as type’ as VTK. Failing to select VTK as the file type may result in an error.


File open
Host: localhost
Path: mfix/tutorials/FluidBed_DES
Filter: *
[✓] Use "current working directory" by default
[ ] Show dot files
File grouping: Smart
Directories:
. (current directory)
.. (go up 1 directory level)
AUTOTEST
Files:
DES_FB1_DES_*.vtp database
(11 total files)
DES_FB1_DES_00000.vtp
DES_FB1_DES_00001.vtp
DES_FB1_DES_00002.vtp
DES_FB1_DES_00003.vtp
DES_FB1_DES_00004.vtp
...
DES_FB1_DES_00006.vtp
DES_FB1_DES_00007.vtp
DES_FB1_DES_00008.vtp
Open file as type: VTK

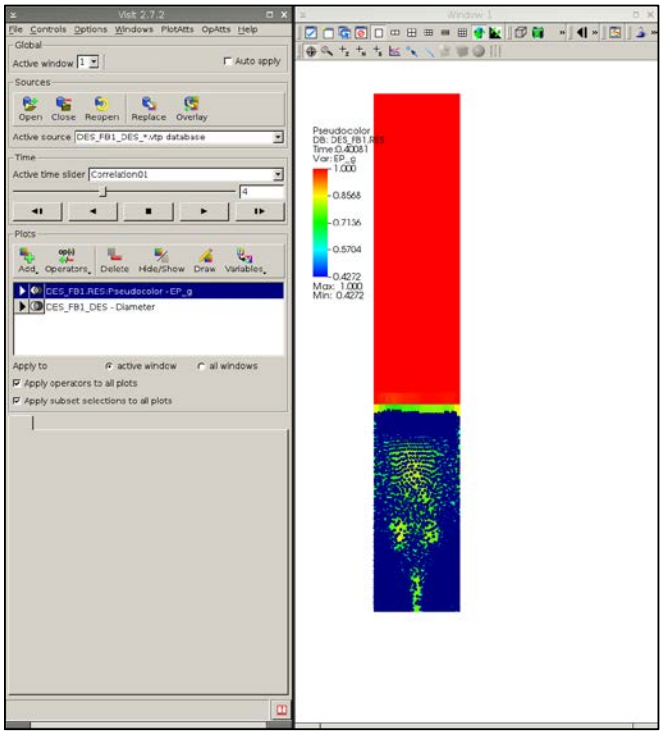


The gas phase volume fraction is plotted by

Add → Molecule → Diameter

Draw Display the particles by clicking the Draw

A dialog to edit the particle display properties is found by selecting:
PlotAtts > Molecule…
It may be necessary to adjust the "Fixed atom radius" to properly display the particles.


VisIt 2.7.2
File Controls Options Windows PlotAtts OpAtts Help
Global
Active window 1
Auto apply
Sources
Open Close Reopen Replace Overlay
Active source DES_FB1_DES_*.vtp database
Time
Active time slider Correlation01
Plots
Add Operators Delete Hide/Show Draw Variables
DES_FB1.RES:Pseudocolor - EP_g
DES_FB1_DES - Diameter
Apply to active window all windows
Apply operators to all plots
Apply subset selections to all plots
Window 1
Pseudocolor
DB: DES_FB1.RES
Time:0.40081
Var: EP_g
1.000
0.8568
0.7136
0.5704
0.4272
Max: 1.000
Min: 0.4272

7 Simulation Units

Simulations can be setup using the International System of Units (SI) or the centimeter-gram-second system (CGS). Although the majority of units are consistent with the specified systems, there are exceptions. The following table provides the SI and CGS units employed by MFIX for various quantities.

Quantity	MFIX SI unit	MFIX CGS unit
length, position	meter (m)	centimeter (cm)
mass	kilogram (kg)	gram (g)
time	second (s)	second (s)
thermal temperature	Kelvin (K)	Kelvin (K)
energy†	Joule (J)	*calorie (cal)*
amount of substance‡	*kilomole (kmol)*	mole (mol)
force	Newton (1 N = 1 kg·m·s^{-2})	dyne (1 dyn = 1 g·cm·s^{-2})
pressure	Pascal (1 Pa = 1 N·m^{-2})	barye (1 Ba = 1 dyn·cm^{-2})
dynamic viscosity	Pa·s	poise (1 P = 1 g·cm^{-1}·s^{-1})
kinematic viscosity	m^2·s^{-1}	Stokes (1 St = 1 cm^2·s^{-1})
gas constant	J·K^{-1}·$kmol^{-1}$	erg·K^{-1}·mol^{-1}
enthalpy	J	cal
specific heat	J·kg^{-1}·K^{-1}	cal·g^{-1}·K^{-1}
thermal conductivity	J·m^{-1}·K^{-1}·s^{-1}	cal·cm^{-1}·K^{-1}·s^{-1}

† The CGS unit for energy is the ergon (1 erg = 1 dyne·cm). This is reflected in MFIX through the gas constant. However, all thermochemical properties related to the energy equations are based in calories for CGS units. Entries in the Burcat database are **always** specified in terms of calories regardless of the simulation units. MFIX converts the entries to joules after reading the database when SI units are used.

‡ The SI unit for the amount of a substance is the mole (mol). These units are needed when specifying reaction rates:

- *amount per time per volume* for Eulerian model reactions
- *amount per time* for Lagrangian model reactions

8 Keywords in Input Data File (mfix.dat)

The symbols used in the table are as follows:

Dimension	Description
1	Cell number in x, y, or z direction
M	Solids-phase number
N	Species number
IC	Initial condition number
BC	Boundary condition number
IS	Internal surface number
USR	User-defined output number

[DEFAULT VALUE] indicates a default value.

8.1 Run Control

This section contains basic run time information. The flags for enabling/disabling various governing equations are provided.

RUN_NAME *Required* CHARACTER

Name used to create output files. The name should generate legal file names after appending extensions. Ex: Given the input, RUN_NAME = "bub01", MFIX will generate the output files: BUB01.LOG, BUB01.OUT, BUB01.RES, etc.

DESCRIPTION CHARACTER

Problem description. Limited to 60 characters.

UNITS *Required* CHARACTER

Simulation input/output units.

CGS -------------------------------- All input and output in CGS units (g, cm, s, cal).
SI ------------------------------------ All input and output in SI units (kg, m, s, J).

RUN_TYPE *Required* CHARACTER

Type of run.

NEW -------------------------------- A new run. There should be no .RES, .SPx, .OUT, or .LOG files in the run directory.
RESTART_1 ---------------------- Traditional restart. The run continues from the last time the .RES file was updated and new data is added to the SPx files.
RESTART_2 ---------------------- Start a new run with initial conditions from a .RES file created from another run. No other data files (SPx) should be in the run directory.

TIME DOUBLE PRECISION

Simulation start time. This is typically zero.

TSTOP DOUBLE PRECISION

Simulation stop time.

DT
DOUBLE PRECISION

Initial time step size. If left undefined, a steady-state calculation is performed.

DT_MAX
DOUBLE PRECISION

Maximum time step size.

DT_MIN
DOUBLE PRECISION

Minimum time step size.

DT_FAC
DOUBLE PRECISION

Factor for adjusting time step. * The value must be less than or equal to 1.0. * A value of 1.0 keeps the time step constant which may help overcome initial non-convergence.

PERSISTENT_MODE
LOGICAL

Force a forward time-step if the maximum number of iterations, MAX_NIT, is reached. The forward time-step is only forced after reaching the minimum time-step, DT_MIN, for adjustable time-step simulations (DT_FAC /= 1). This option should be used with caution as unconverged time-steps may lead to poor simulation results and/or additional convergence issues.

.TRUE. ---------------------------- Force forward time-step when DT=DT_MIN and the maximum number of iterations are reached.
[*.FALSE.*] -------------------------- Abort run when DT < DT_MIN.

AUTO_RESTART
LOGICAL

Flag to restart the code when DT < DT_MIN.

MOMENTUM_X_EQ(Phase)
LOGICAL

Flag to enable/disable solving the X-momentum equations.

[*.TRUE.*] --------------------------- Solve X-momentum equations.
.FALSE. ---------------------------- The X velocity initial conditions persist throughout the simulation.

MOMENTUM_Y_EQ(Phase)
LOGICAL

Flag to enable/disable solving the Y-momentum equations.

[*.TRUE.*] --------------------------- Solve Y-momentum equations.
.FALSE. ---------------------------- The Y velocity initial conditions persist throughout the simulation.

MOMENTUM_Z_EQ(Phase)
LOGICAL

Flag to enable/disable solving the Z-momentum equations.

[*.TRUE.*] --------------------------- Solve Z-momentum equations.
.FALSE. ---------------------------- The Z velocity initial conditions persist throughout the simulation.

JACKSON
LOGICAL

Flag to enable Jackson form of momentum equations. See Anderson and Jackson, (1967), IECF, 6(4), p.527.

.TRUE. ----------------------------- Solve Jackson form of momentum equations.
[*.FALSE.*] -------------------------- Default form.

ISHII

LOGICAL

Flag to enable Ishii form of momentum equations. See Ishii, (1975), Thermo-fluid dynamic theory of two-phase flow.

.TRUE. ----------------------------	Solve Ishii form of momentum equations.
[*.FALSE.*] --------------------------	Default form.

ENERGY_EQ

LOGICAL

Solve energy equations.

[*.TRUE.*] ---------------------------	Solve energy equations.
.FALSE. ---------------------------	Do not solve energy equations.

SPECIES_EQ(Phase)

LOGICAL

Solve species transport equations.

[*.TRUE.*] ---------------------------	Solve species equations.
.FALSE. ---------------------------	Do not solve species equations.

GRANULAR_ENERGY

LOGICAL

Granular energy formulation selection.

Applies to solids models: TFM

[*.FALSE.*] --------------------------	Use algebraic granular energy equation formulation.
.TRUE. ----------------------------	Use granular energy transport equation (PDE) formulation.

K_EPSILON

LOGICAL

The K-Epsilon turbulence model (for single-phase flow).

- Numerical parameters (eg under-relaxation) are the same as the ones for SCALAR (index = 9).
- All walls must be defined (NSW, FSW or PSW) in order to use standard wall functions. If a user does not specify a wall type, the simulation will not contain the typical turbulent profile in wall-bounded flows.

.TRUE. ----------------------------	Enable the K-epsilon turbulence model (for single-phase flow) using standard wall functions.
[*.FALSE.*] --------------------------	Do not use K-epsilon turbulence model

L_SCALE0

DOUBLE PRECISION

Value of turbulent length initialized. This may be overwritten in specific regions with the keyword IC_L_SCALE.

MU_GMAX

DOUBLE PRECISION

Maximum value of the turbulent viscosity of the fluid, which must be defined if any turbulence model is used. A value MU_GMAX =1.E+03 is recommended. (see calc_mu_g.f)

DRAG_TYPE

CHARACTER

Available gas-solids drag models. Note: The extension _PCF following the specified drag model indicates that the polydisperse correction factor is available. For PCF details see:

- Van der Hoef MA, Beetstra R, Kuipers JAM. (2005) Journal of Fluid Mechanics.528:233-254.
- Beetstra, R., van der Hoef, M. A., Kuipers, J.A.M. (2007). AIChE Journal, 53:489-501.
- Erratum (2007), AIChE Journal, Volume 53:3020

SYAM_OBRIEN ------------------	Syamlal M, OBrien TJ (1988). International Journal of Multiphase Flow 14:473-481. Two additional parameters may be specified: DRAG_C1, DRAG_D1
GIDASPOW -----------------------	Ding J, Gidaspow D (1990). AIChE Journal 36:523-538
GIDASPOW_BLEND -----------	Lathouwers D, Bellan J (2000). Proceedings of the 2000 U.S. DOE Hydrogen Program Review NREL/CP-570-28890.
WEN_YU --------------------------	Wen CY, Yu YH (1966). Chemical Engineering Progress Symposium Series 62:100-111.
KOCH_HILL ----------------------	Hill RJ, Koch DL, Ladd JC (2001). Journal of Fluid Mechanics, 448: 213-241. and 448:243-278.
BVK --------------------------------	Beetstra, van der Hoef, Kuipers (2007). Chemical Engineering Science 62:246-255
HYS --------------------------------	Yin, X, Sundaresan, S. (2009). AIChE Journal 55:1352-1368 This model has a lubrication cutoff distance, LAM_HYS, that can be specified.
USER_DRAG --------------------	Invoke user-defined drag law. (usr_drag.f)
GIDASPOW_PCF ---------------	see GIDASPOW
GIDASPOW_BLEND_PCF ----	see GIDASPOW_BLEND
WEN_YU_PCF ------------------	see WEN_YU
KOCH_HILL_PCF ---------------	see KOCH_HILL

DRAG_C1

DOUBLE PRECISION

Quantity for calibrating Syamlal-O'Brien drag correlation using Umf data. This is determined using the Umf spreadsheet.

DRAG_D1

DOUBLE PRECISION

Quantity for calibrating Syamlal-O'Brien drag correlation using Umf data. This is determined using the Umf spreadsheet.

LAM_HYS

DOUBLE PRECISION

The lubrication cutoff distance for HYS drag model. In practice this number should be on the order of the mean free path of the gas for smooth particles, or the RMS roughness of a particle if they are rough (if particle roughness is larger than the mean free path).

SUBGRID_TYPE

CHARACTER

Subgrid models.

Applies to solids models: TFM

IGCI --------------------------------	Igci, Y., Pannala, S., Benyahia, S., and Sundaresan S. (2012). Industrial & Engineering Chemistry Research, 2012, 51(4):2094-2103
MILIOLI ----------------------------	Milioli, C.C., Milioli, F. E., Holloway, W., Agrawal, K. and Sundaresan, S. (2013). AIChE Journal, 59:3265-3275.

FILTER_SIZE_RATIO DOUBLE PRECISION

Ratio of filter size to computational cell size.

Applies to solids models: TFM

SUBGRID_WALL LOGICAL

Flag for subgrid wall correction.

Applies to solids models: TFM

[*.FALSE.*] -------------------------- Do not include wall correction.

.TRUE. ---------------------------- Include subgrid wall correction.

MODEL_B LOGICAL

Shared gas-pressure formulation. See Syamlal, M. and Pannala, S. "Multiphase continuum formulation for gas-solids reacting flows," chapter in Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice, S. Pannala, M. Syamlal and T.J. O'Brien (editors), IGI Global, Hershey, PA, 2011.

[*.FALSE.*] -------------------------- Use Model A

.TRUE. ---------------------------- Use Model B. Bouillard, J.X., Lyczkowski, R.W., Folga, S., Gidaspow, D., Berry, G.F. (1989). Canadian Journal of Chemical Engineering 67:218-229.

NSCALAR INTEGER

The number of user-defined scalar transport equations to solve.

PHASE4SCALAR(Scalar Equation) INTEGER

The phase convecting the indexed scalar transport equation.

8.2 Physical Parameters

P_REF DOUBLE PRECISION

Reference pressure [0.0].

P_SCALE DOUBLE PRECISION

Scale factor for pressure [1.0].

GRAVITY DOUBLE PRECISION

Gravitational acceleration [980.7 in CGS; 9.87 in SI].

GRAVITY_X DOUBLE PRECISION

X-component of gravitational acceleration vector.
By default, the gravity force acts in the negative y-direction.

GRAVITY_Y DOUBLE PRECISION

Y-component of gravitational acceleration vector.
By default, the gravity force acts in the negative y-direction.

GRAVITY_Z
DOUBLE PRECISION

Z-component of gravitational acceleration vector.
By default, the gravity force acts in the negative y-direction.

8.3 Numerical Parameters

This section contains keywords for defining numerical parameters. Keywords related to solving the governing equations (e.g., LEQ_IT, DISCRETIZE, UR_FAC, etc.) are dimensioned for the ten types of equations:

Index	Equation Type
1	Gas Pressure
2	Solids Volume Fraction
3	Gas and Solids U Momentum Equation
4	Gas and Solids V Momentum Equation
5	Gas and Solids W Momentum Equation
6	Gas and Solids Energy Equations (Temperature)
7	Gas and Solids Species Mass Fractions
8	Granular Temperature
9	User-Defined Scalar and K-Epsilon Equation
10	DES Diffusion Equation

For example, LEQ_IT(3) = 10, specifies to use 10 iterations within the linear equation solver for the U Momentum Equations (of type 3).

MAX_NIT
INTEGER

Maximum number of iterations [500].

NORM_G
DOUBLE PRECISION

Factor to normalize the gas continuity equation residual. The residual from the first iteration is used if NORM_G is left undefined. NORM_G=0 invokes a normalization method based on the dominant term in the continuity equation. This setting may speed up calculations, especially near a steady state and incompressible fluids. But, the number of iterations for the gas phase pressure should be increased, LEQ_IT(1), to ensure mass balance

NORM_S
DOUBLE PRECISION

Factor to normalize the solids continuity equation residual. The residual from the first iteration is used if NORM_S is left undefined. NORM_S = 0 invokes a normalization method based on the dominant term in the continuity equation. This setting may speed up calculations, especially near a steady state and incompressible fluids. But, the number of iterations for the solids volume fraction should be increased, LEQ_IT(2), to ensure mass balance.

TOL_RESID
DOUBLE PRECISION

Maximum residual at convergence (Continuity + Momentum) [1.0d-3].

TOL_RESID_T
DOUBLE PRECISION

Maximum residual at convergence (Energy) [1.0d-4].

TOL_RESID_X
DOUBLE PRECISION

Maximum residual at convergence (Species Balance) [1.0d-4].

TOL_RESID_TH
DOUBLE PRECISION

Maximum residual at convergence (Granular Energy) [1.0d-4].

TOL_RESID_SCALAR
DOUBLE PRECISION

Maximum residual at convergence (Scalar Equations) [1.0d-4].

TOL_RESID_K_EPSILON
DOUBLE PRECISION

Maximum residual at convergence (K_Epsilon Model) [1.0d-4].

TOL_DIVERGE
DOUBLE PRECISION

Minimum residual for declaring divergence [1.0d+4]. This parameter is useful for incompressible fluid simulations because velocity residuals can take large values for the second iteration (e.g., 1e+8) before dropping down to smaller values for the third iteration.

DETECT_STALL
LOGICAL

Reduce the time step if the residuals stop decreasing. Disabling this feature may help overcome initial non-convergence.

.FALSE. ---------------------------- Continue iterating if residuals stall.
[*.TRUE.*] --------------------------- Reduce time step if residuals stall.

LEQ_METHOD(Equation ID Number)
INTEGER

LEQ Solver selection. BiCGSTAB is the default method for all equation types.

1 ------------------------------------- SOR - Successive over-relaxation
[*2*] ----------------------------------- BiCGSTAB - Biconjugate gradient stabilized.
3 ------------------------------------- GMRES - Generalized minimal residual method
5 ------------------------------------- CG - Conjugate gradient

LEQ_TOL(Equation ID Number)
DOUBLE PRECISION

Linear Equation tolerance [1.0d-4].

LEQ_IT(Equation ID Number)
INTEGER

Number of iterations in the linear equation solver.

- 20 iterations for equation types 1-2
- 5 iterations for equation types 3-5,10
- 15 iterations for equation types 6-9

LEQ_SWEEP(Equation ID Number)

CHARACTER

Linear equation sweep direction. This applies when using GMRES or when using the LINE preconditioner with BiCGSTAB or CG methods. 'RSRS' is the default for all equation types.

RSRS	(Red/Black Sweep, Send Receive) repeated twice
ISIS	(Sweep in I, Send Receive) repeated twice
JSJS	(Sweep in J, Send Receive) repeated twice
KSKS	(Sweep in K, Send Receive) repeated twice
ASAS	(All Sweep, Send Receive) repeated twice

LEQ_PC(Equation ID Number)

CHARACTER

Linear precondition used by the BiCGSTAB and CG LEQ solvers. 'LINE' is the default for all equation types.

NONE	No preconditioner
LINE	Line relaxation
DIAG	Diagonal Scaling

UR_FAC(Equation ID Number)

DOUBLE PRECISION

Under relaxation factors.

- 0.8 for equation types 1,9
- 0.5 for equation types 2,3,4,5,8
- 1.0 for equation types 6,7,10

UR_F_GS

DOUBLE PRECISION

The implicitness calculation of the gas-solids drag coefficient may be underrelaxed by changing ur_f_gs, which takes values between 0 to 1.

- 0 updates F_GS every time step
- 1 updates F_GS every iteration

UR_KTH_SML

DOUBLE PRECISION

Under relaxation factor for conductivity coefficient associated with other solids phases for IA Theory [1.0].

DISCRETIZE(Equation ID Number)

INTEGER

Discretization scheme of equations.

[*0*]	First-order upwinding.
1	First-order upwinding (using down-wind factors).
3	Smart.
2	Superbee (recommended method).
5	QUICKEST (does not work).
4	ULTRA-QUICK.
7	van Leer.
6	MUSCL.
8	minmod.
9	Central (often unstable; useful for testing).

DEF_COR
LOGICAL

Use deferred correction method for implementing higher order discretization.

[*.FALSE.*] -------------------------	Use down-wind factor method (default).
.TRUE. ----------------------------	Use deferred correction method.

CHI_SCHEME
LOGICAL

This scheme guarantees that the set of differenced species mass balance equations maintain the property that the sum of species mass fractions sum to one. This property is not guaranteed when a flux limiter is used with higher order spatial discretization schemes. Note: The chi-scheme is implemented for SMART and MUSCL discretization schemes. Darwish, M.S., Moukalled, F. (2003). Computer Methods in Applied Mech. Eng., 192(13):1711-1730.

[*.FALSE.*] -------------------------	Do not use the chi-scheme.
.TRUE. ----------------------------	Use the chi-scheme correction.

FPFOI
LOGICAL

Four point fourth order interpolation and is upstream biased. Notes:

- DISCRETIZE(*) defaults to Superbee if this scheme is chosen and DISCRETIZE(*) < 2.
- Set C_FAC between 0 and 1 when using this scheme.

[*.FALSE.*] -------------------------	Do not use fourth order interpolation.
.TRUE. ----------------------------	Use fourth order interpolation.

C_FAC
DOUBLE PRECISION

Factor between zero and one used in the universal limiter when using four point, fourth order interpolation (FPFOI).

- Choosing one gives (diffusive) first order upwinding.
- The scheme becomes more compressive as values near zero.

CN_ON
LOGICAL

Temporal discretization scheme.

[*.FALSE.*] -------------------------	Implicit Euler based temporal discretization scheme employed (first order accurate in time).
.TRUE. ----------------------------	Two-step implicit Runge-Kutta method based temporal discretization scheme employed. This method should be second order accurate in time excluding pressure terms and restart time step which are first order accurate. However, recent testing shows that second order accuracy in time is not observed.

MAX_INLET_VEL_FAC
DOUBLE PRECISION

The code declares divergence if the velocity anywhere in the domain exceeds a maximum value. This maximum value is automatically determined from the boundary values. The user may scale the maximum value by adjusting this scale factor [1.0d0].

DO_TRANSPOSE
LOGICAL

Solve transpose of linear system. (BICGSTAB ONLY).

ICHECK_BICGS
INTEGER

Frequency to check for convergence. (BICGSTAB ONLY)

OPT_PARALLEL LOGICAL

Sets optimal LEQ flags for parallel runs.

USE_DOLOOP LOGICAL

Use do-loop assignment over direct vector assignment.

IS_SERIAL LOGICAL

Calculate dot-products more efficiently (Serial runs only.)

8.4 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.

8.4.1 Basic Geometry

This section contains keywords to specify the domain bounds and spatial discretization.

COORDINATES CHARACTER

Coordinates used in the simulation.

CARTESIAN	---------------------- Cartesian coordinates.
CYLINDRICAL	------------------- Cylindrical coordinates.

IMAX INTEGER

Number of cells in the x (r) direction.

DX(Cell) DOUBLE PRECISION

Cell sizes in the x (r) direction. Enter values from DX(0) to DX(IMAX-1).

- Use uniform mesh size with higher-order discretization methods.
- DX should be kept uniform in cylindrical coordinates for strict momentum conservation.

XMIN DOUBLE PRECISION

The inner radius in the simulation of an annular cylindrical region.

XLENGTH DOUBLE PRECISION

Reactor length in the x (r) direction.

JMAX INTEGER

Number of cells in the y-direction.

DY(Cell) DOUBLE PRECISION

Cell sizes in the y-direction. Enter values from DY(0) to DY(IMAX-1). Use uniform mesh size with second-order discretization methods.

YLENGTH
DOUBLE PRECISION

Reactor length in the y-direction.

NO_K
LOGICAL

Flag to disable the third dimension (i.e., 2D simulation).
- Z axis in Cartesian coordinate system
- Theta in Cylindrical coordinate system

[*.FALSE.*] -------------------------- 3D simulation.
.TRUE. ----------------------------- 2D simulation.

KMAX
INTEGER

Number of cells in the z-direction.

DZ(Cell)
DOUBLE PRECISION

Cell sizes in the z (theta) direction. Enter values from DZ(0) to DZ(IMAX-1). Use uniform mesh size with second-order discretization methods.

ZLENGTH
DOUBLE PRECISION

Reactor length in the z (theta) direction.

CYCLIC_X
LOGICAL

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
LOGICAL

Flag for making the x-direction cyclic with pressure drop. If the keyword FLUX_G is given a value this becomes a cyclic boundary condition with specified mass flux. 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
DOUBLE PRECISION

Fluid pressure drop across XLENGTH when a cyclic boundary condition with pressure drop is imposed in the x-direction.

CYCLIC_Y
LOGICAL

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

LOGICAL

Flag for making the y-direction cyclic with pressure drop. If the keyword FLUX_G is given a value this becomes a cyclic boundary condition with specified mass flux. 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

DOUBLE PRECISION

Fluid pressure drop across YLENGTH when a cyclic boundary condition with pressure drop is imposed in the y-direction.

CYCLIC_Z

LOGICAL

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

LOGICAL

Flag for making the z-direction cyclic with pressure drop. If the keyword FLUX_G is given a value this becomes a cyclic boundary condition with specified mass flux. 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

DOUBLE PRECISION

Fluid pressure drop across ZLENGTH when a cyclic boundary condition with pressure drop is imposed in the z-direction.

SHEAR

LOGICAL

Imposes a mean shear on the flow field as a linear function of the x coordinate. This feature should only be used when CYCLIC_X is .TRUE. and the keyword V_SH is set.

V_SH

DOUBLE PRECISION

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.

FLUX_G

DOUBLE PRECISION

If a value is specified (in units of g/cm^2.s), the domain-averaged gas flux is held constant at that value in simulations over a periodic domain. A pair of boundaries specified as periodic with fixed pressure drop is then treated as periodic with fixed mass flux. Even for this case a pressure drop must also be specified, which is used as the initial guess in the simulations.

CYLINDRICAL_2D

LOGICAL

Applies the 2.5D model for cylindrical column by combining 2D assumption and axi-symmetric assumption. Li et al. (2015). A 2.5D computational method to simulate cylindrical fluidized beds, Chemical Engineering Science, 123:236-246.

I_CYL_NUM
INTEGER

Parameter to control the plate half width and the wedge radius in the 2.5D cylindrical model. This value should be less than half the grid cells in the radial direction (IMAX/2). [1]

I_CYL_TRANSITION
INTEGER

Parameter to smooth the transition from cylindrical to 2D in the 2.5D cylindrical model. [2]

[2]	Two cell smoothing transition.
1	One cell smoothing transition.
0	No smoothing.

CPX
DOUBLE PRECISION

Location of control points in x-direction.

NCX
INTEGER

Number of cells within a segment (x-direction).

ERX
DOUBLE PRECISION

Expansion ratio (last DX/first DX) in a segment (x-direction).

FIRST_DX
DOUBLE PRECISION

Value of first DX in a segment (x-direction). A negative value will copy DX from previous segment (if available).

LAST_DX
DOUBLE PRECISION

Value of last DX in a segment (x-direction). A negative value will copy DX from next segment (if available).

CPY
DOUBLE PRECISION

Location of control points in y-direction.

NCY
INTEGER

Number of cells within a segment (y-direction).

ERY
DOUBLE PRECISION

Expansion ratio (last DY/first DY) in a segment (y-direction).

FIRST_DY
DOUBLE PRECISION

Value of first DY in a segment (y-direction). A negative value will copy DY from previous segment (if available).

LAST_DY
DOUBLE PRECISION

Value of last DY in a segment (y-direction). A negative value will copy DY from next segment (if available).

CPZ
DOUBLE PRECISION

Location of control points in z-direction.

NCZ INTEGER

Number of cells within a segment (z-direction).

ERZ DOUBLE PRECISION

Expansion ratio (last DZ/first DZ) in a segment (z-direction).

FIRST_DZ DOUBLE PRECISION

Value of first DZ in a segment (z-direction). A negative value will copy DZ from previous segment (if available).

LAST_DZ DOUBLE PRECISION

Value of last DZ in a segment (z-direction). A negative value will copy DZ from next segment (if available).

8.4.2 Cartesian Grid

The Cartesian grid cut-cell technique has been implemented in MFIX, which allows the definition of curved or sloping boundaries, instead of the usual stair-step representation. Computational cells are truncated at the wall to conform to the shape of the boundaries. When a face is truncated, the velocity node is moved to the center of the face. The cell truncation introduces an additional face, called the cut face. Face surface areas and cell volumes are updated based on the shape of the cut cell. The contribution of the new cut face is added to the computation. The data can be saved in a vtk file for post-processing purpose.
A detailed user guide named Cartesian_grid_user_guide.pdf is located in mfix-2016.1/doc directory. It should be read prior to utilizing the Cartesian grid feature.

CARTESIAN_GRID LOGICAL

Activate Cartesian grid cut cell technique.

[*.FALSE.*] ------------------------- Do not use Cartesian grid cut cell technique.
.TRUE. ---------------------------- Use Cartesian grid cut cell technique. one of the following methods must be used to define the geometry:

N_QUADRIC INTEGER

Number of quadric surfaces defining the boundaries (<=100).

USE_STL LOGICAL

Use STL file to describe geometry.

[*.FALSE.*] ------------------------- Do not use STL file.
.TRUE. ---------------------------- Read triangulated geometry (for 3d geometry only) from geometry.stl.

USE_MSH LOGICAL

Use .msh file to describe geometry.

[*.FALSE.*] ------------------------- Do not use .msh file.
.TRUE. ---------------------------- Read geometry (for 3d geometry only) from geometry.msh.

QUADRIC_FORM(Quadric ID)

CHARACTER

Form of the quadric surface equation.

NORMAL	Use normal form, as defined in equation (1). The LAMDBA\
PLANE	Plane. Needs to define N_X,N_Y,N_Z (unit normal vector pointing away from fluid cells).
X_CYL_INT	Cylinder aligned with x-axis, internal flow. Needs to define RADIUS(QID).
X_CYL_EXT	Cylinder aligned with x-axis, external flow. Needs to define RADIUS(QID).
Y_CYL_INT	Cylinder aligned with y-axis, internal flow. Needs to define RADIUS(QID).
Y_CYL_EXT	Cylinder aligned with y-axis, external flow. Needs to define RADIUS(QID).
Z_CYL_INT	Cylinder aligned with z-axis, internal flow. Needs to define RADIUS(QID).
Z_CYL_EXT	Cylinder aligned with z-axis, external flow. Needs to define RADIUS(QID).
X_CONE	Cone aligned with x-axis, internal flow. Needs to define HALF_ANGLE(QID).
Y_CONE	Cone aligned with y-axis, internal flow. Needs to define HALF_ANGLE(QID).
Z_CONE	Cone aligned with z-axis, internal flow. Needs to define HALF_ANGLE(QID).
SPHERE_INT	Sphere, internal flow. Needs to define RADIUS(QID).
SPHERE_EXT	Sphere, external flow. Needs to define RADIUS(QID).
C2C	Cylinder-to-cylinder conical junction, internal flow. Needs to be defined between two cylinders.
TORUS_INT	Torus, internal flow. Needs to define TORUS_R1(QID) and TORUS_R2(QID).A torus is not a quadric surface but is defined as a basic shape.
TORUS_EXT	Torus, external flow. Needs to define TORUS_R1(QID) and TORUS_R2(QID).
Y_UCOIL_EXT	Pair of parallel cylinders (y-direction), capped at both ends by a cylinder at 90 degree angle to create a U-shaped coil. Needs UCOIL_R1, UCOIL_R2, UCOIL_Y1, UCOIL_Y2.
XY_BEND_INT	Bend between two cylinders in the XY plane, Needs BEND_R1,BEND_R2,BEND_THETA1,BEND_THETA2.
Y_C2C_INT	connects two vertical cylinders by a conical section. Needs C2C_R1,C2C_R2,C2C_Y1,C2C_Y2.
REACTOR1	Reactor, made of two vertical cylinders, connected by a conical section.Each cylinder is rounded and closed by a conical cap. Needs REACTOR1_R1,REACTOR1_R2,REACTOR1_Y1,REACTOR1_Y2, REACTOR1_YR1,REACTOR1_YR2,REACTOR1_RR1,REACTOR1_RR2, REACTOR1_THETA1,REACTOR1_THETA2.

QUADRIC_SCALE

DOUBLE PRECISION

Scaling factor, applied to all quadric geometry parameters. Must be a positive number.

USE_POLYGON
LOGICAL

Use polygons to describe geometry.

[*.FALSE.*] -------------------------- Do not use polygons.

.TRUE. ----------------------------- Read polygon data (for 2d geometry only) from poly.dat.

N_USR_DEF
INTEGER

Number of user-defined functions (currently limited to 0 or 1). If set to 1, the geometry is defined in the user subroutine eval_usr_fct.f.

[*0*] ------------------------------------ Do not use user-defined function

1 ------------------------------------- Use one user-defined function

LAMBDA_X(Quadric ID)
DOUBLE PRECISION

Coefficient LAMBDA_X in equation (1) ('NORMAL' form) or x-component of normal vector defining plane in equation (5) ('DEGENERATE' form).

LAMBDA_Y(Quadric ID)
DOUBLE PRECISION

Coefficient LAMBDA_Y in equation (1) ('NORMAL' form) or y-component of normal vector defining plane in equation (5) ('DEGENERATE' form).

LAMBDA_Z(Quadric ID)
DOUBLE PRECISION

Coefficient LAMBDA_Z in equation (1) ('NORMAL' form) or z-component of normal vector defining plane in equation (5) ('DEGENERATE' form).

DQUADRIC(Quadric ID)
DOUBLE PRECISION

Coefficient D in equation (1).

THETA_X(Quadric ID)
DOUBLE PRECISION

Rotation angle with respect to x-axis (degrees).

THETA_Y(Quadric ID)
DOUBLE PRECISION

Rotation angle with respect to y-axis (degrees).

THETA_Z(Quadric ID)
DOUBLE PRECISION

Rotation angle with respect to z-axis (degrees).

RADIUS(Quadric ID)
DOUBLE PRECISION

Cylinder radius (used when QUADRIC_FORM = *_CYL_***)

HALF_ANGLE(Quadric ID)
DOUBLE PRECISION

Cone half angle, expressed in degrees (used when QUADRIC_FORM = *_CONE)

TORUS_R1(Quadric ID)
DOUBLE PRECISION

Torus Radius 1 (used when QUADRIC_FORM = TORUS_*), R1>R2 for a ring.

TORUS_R2(Quadric ID)
DOUBLE PRECISION

Torus Radius 2 (used when QUADRIC_FORM = TORUS_*), R1>R2 for a ring.

UCOIL_R1(Quadric ID) DOUBLE PRECISION
U-shaped coil Radius 1 (used when QUADRIC_FORM = UCOIL*), UCOIL_R1>UCOIL_R2.

UCOIL_R2(Quadric ID) DOUBLE PRECISION
U-shaped coil Radius 2 (used when QUADRIC_FORM = UCOIL*), UCOIL_R1>UCOIL_R2.

UCOIL_Y1(Quadric ID) CHARACTER
U-shaped coil ymax (used when QUADRIC_FORM = UCOIL*), UCOIL_Y2>UCOIL_Y1.

UCOIL_Y2(Quadric ID) DOUBLE PRECISION
U-shaped coil ymin (used when QUADRIC_FORM = UCOIL*), UCOIL_Y2>UCOIL_Y1.

BEND_R1(Quadric ID) DOUBLE PRECISION
Bend Radius 1 (used when QUADRIC_FORM = BEND*), BEND_R1>BEND_R2.

BEND_R2(Quadric ID) DOUBLE PRECISION
Bend Radius 2 (used when QUADRIC_FORM = BEND*), BEND_R1>BEND_R2.

BEND_THETA1(Quadric ID) DOUBLE PRECISION
Bend start angle, in degrees (used when QUADRIC_FORM = BEND*).

BEND_THETA2(Quadric ID) DOUBLE PRECISION
Bend end angle, in degrees (used when QUADRIC_FORM = BEND*).

C2C_R1(Quadric ID) DOUBLE PRECISION
Cylinder-cone_cylinder Radius 1 (used when QUADRIC_FORM = C2C*).

C2C_R2(Quadric ID) DOUBLE PRECISION
Cylinder-cone_cylinder Radius 2 (used when QUADRIC_FORM = C2C*).

C2C_Y1(Quadric ID) CHARACTER
Cylinder-cone_cylinder Y1 (used when QUADRIC_FORM = C2C*). If Y1=Y2, then R1=R2.

C2C_Y2(Quadric ID) DOUBLE PRECISION
Cylinder-cone_cylinder Y2 (used when QUADRIC_FORM = C2C*). If Y1=Y2, then R1=R2.

REACTOR1_R1(Quadric ID) DOUBLE PRECISION
Reactor 1, lower cylinder radius.

REACTOR1_R2(Quadric ID) DOUBLE PRECISION
Reactor 1, upper cylinder radius.

REACTOR1_Y1(Quadric ID) DOUBLE PRECISION
Reactor 1, lower conical transition between cylinders.

REACTOR1_Y2(Quadric ID) Reactor 1, upper conical transition between cylinders.	DOUBLE PRECISION
REACTOR1_YR1(Quadric ID) Reactor 1, lower rounding below cylinder.	DOUBLE PRECISION
REACTOR1_YR2(Quadric ID) Reactor 1, upper rounding above cylinder.	DOUBLE PRECISION
REACTOR1_RR1(Quadric ID) Reactor 1, lower rounding radius.	DOUBLE PRECISION
REACTOR1_RR2(Quadric ID) Reactor 1, upper rounding radius.	DOUBLE PRECISION
REACTOR1_THETA1(Quadric ID) Reactor 1, lower rounding angle (degrees).	DOUBLE PRECISION
REACTOR1_THETA2(Quadric ID) Reactor 1, upper rounding angle (degrees).	DOUBLE PRECISION
N_X(Quadric ID) X-component of normal vector defining the plane (used when QUADRIC_FORM = PLANE).	DOUBLE PRECISION
N_Y(Quadric ID) Y-component of normal vector defining the plane (used when QUADRIC_FORM = PLANE).	DOUBLE PRECISION
N_Z(Quadric ID) Z-component of normal vector defining the plane (used when QUADRIC_FORM = PLANE).	DOUBLE PRECISION
T_X(Quadric ID) Translation in x-direction.	DOUBLE PRECISION
T_Y(Quadric ID) Translation in y-direction.	DOUBLE PRECISION
T_Z(Quadric ID) Translation in z-direction.	DOUBLE PRECISION
CLIP_XMIN(Quadric ID) Lower x-limit where the quadric is defined.	DOUBLE PRECISION
CLIP_XMAX(Quadric ID) Upper x-limit where the quadric is defined.	DOUBLE PRECISION

CLIP_YMIN(Quadric ID) DOUBLE PRECISION

Lower y-limit where the quadric is defined.

CLIP_YMAX(Quadric ID) DOUBLE PRECISION

Upper y-limit where the quadric is defined.

CLIP_ZMIN(Quadric ID) DOUBLE PRECISION

Lower z-limit where the quadric is defined.

CLIP_ZMAX(Quadric ID) DOUBLE PRECISION

Upper z-limit where the quadric is defined.

PIECE_XMIN(Quadric ID) DOUBLE PRECISION

Lower x-limit where the quadric is defined in a piecewise group.

PIECE_XMAX(Quadric ID) DOUBLE PRECISION

Upper z-limit where the quadric is defined in a piecewise group.

PIECE_YMIN(Quadric ID) DOUBLE PRECISION

Lower y-limit where the quadric is defined in a piecewise group.

PIECE_YMAX(Quadric ID) DOUBLE PRECISION

Upper y-limit where the quadric is defined in a piecewise group.

PIECE_ZMIN(Quadric ID) DOUBLE PRECISION

Lower z-limit where the quadric is defined in a piecewise group.

PIECE_ZMAX(Quadric ID) DOUBLE PRECISION

Upper z-limit where the quadric is defined in a piecewise group.

FLUID_IN_CLIPPED_REGION(Quadric ID) LOGICAL

Flag defining the type of cells that are outside of the zone defined by [CLIP_XMIN; CLIP_XMAX], [CLIP_YMIN; CLIP_YMAX], [CLIP_ZMIN; CLIP_ZMAX].

.FALSE.	---------------------------- Remove cells from computational domain.
[*.TRUE.*]	---------------------------- Treat cells as fluid cells.

BC_ID_Q(Quadric ID) INTEGER

Boundary condition flag.

N_GROUP INTEGER

Number of group(s) of quadrics (<=50).

GROUP_SIZE INTEGER

Number of quadrics in the group.

GROUP_Q
INTEGER

Quadric ID assigned to a group.

GROUP_RELATION
CHARACTER

Relation among quadrics of a same group.

OR ----------------------------------	A point belongs to the computational domain if at least one of f(x,y,z) among all quadrics is negative.
AND --------------------------------	A point belongs to the computational domain if all of f(x,y,z) among all quadrics are negative.

RELATION_WITH_PREVIOUS
CHARACTER

Relation between current group and combination of all previous groups.

OR ----------------------------------	A point belongs to the computational domain if f-value for the current group or f-value for the combination of previous groups is negative.
AND --------------------------------	A point belongs to the computational domain if f-value for the current group and f-value for the combination of previous groups is negative.

TOL_SNAP
DOUBLE PRECISION

Tolerance used to snap an intersection point onto an existing cell corner (expressed as a fraction of edge length, between 0.0 and 0.5). For stretched grids, three values can be entered in the x, y and z directions.

TOL_DELH
DOUBLE PRECISION

Tolerance used to limit acceptable values of normal distance to the wall (expressed as a fraction of cell diagonal, between 0.0 and 1.0).

TOL_SMALL_CELL
DOUBLE PRECISION

Tolerance used to detect small cells (expressed as a fraction of cell volume, between 0.0 and 1.0).

TOL_MERGE
DOUBLE PRECISION

Tolerance used to remove duplicate nodes (expressed as a fraction of cell diagonal, between 0.0 and 1.0).

TOL_SMALL_AREA
DOUBLE PRECISION

Tolerance used to detect small faces (expressed as a fraction of original face area, between 0.0 and 1.0).

ALPHA_MAX
DOUBLE PRECISION

Maximum acceptable value of interpolation correction factor.

TOL_F
DOUBLE PRECISION

Tolerance used to find intersection of quadric surfaces or user-defined function with background grid.

TOL_POLY
DOUBLE PRECISION

Tolerance used to find intersection of polygon with background grid.

ITERMAX_INT
INTEGER

Maximum number of iterations used to find intersection points.

TOL_STL
DOUBLE PRECISION

Tolerance used to find intersection of STL triangles with background grid.

STL_SMALL_ANGLE
DOUBLE PRECISION

Smallest angle accepted for valid STL triangles (in degrees). Triangles having an angle smaller that this value will be ignored.

TOL_STL_DP
DOUBLE PRECISION

Dot product tolerance when determining if a point lies in a facet.

DIM_FACETS_PER_CELL
INTEGER

Maximum number of STL facets per cell.

OUT_STL_VALUE
DOUBLE PRECISION

Defines value of F_STL outside of the STL geometry. a value of 1.0 means the domain outside of the STL geometry is excluded from computation, i.e., an internal flow is computed.

-1.0 --------------------------------- model an external flow
[*1.0*] -------------------------------- model an internal flow

STL_BC_ID
INTEGER

Boundary condition flag for the STL geometry

TX_STL
DOUBLE PRECISION

Translation in x-direction, applied to the STL geometry.

TY_STL
DOUBLE PRECISION

Translation in y-direction, applied to the STL geometry.

TZ_STL
DOUBLE PRECISION

Translation in z-direction, applied to the STL geometry.

SCALE_STL
DOUBLE PRECISION

Scaling factor, applied to the STL geometry. Note that translation occurs after scaling.

TOL_MSH
DOUBLE PRECISION

Tolerance used to find intersection of .msh file with background grid.

OUT_MSH_VALUE
DOUBLE PRECISION

Defines value of f outside of the .msh geometry. a value of 1.0 means the domain outside of the .msh geometry is excluded from computation, i.e., an internal flow is computed.

-1.0 --------------------------------- model an external flow
[*1.0*] -------------------------------- model an internal flow

TX_MSH
DOUBLE PRECISION

Translation in x-direction, applied to the .msh geometry.

TY_MSH
DOUBLE PRECISION

Translation in y-direction, applied to the .msh geometry.

TZ_MSH
DOUBLE PRECISION

Translation in z-direction, applied to the .msh geometry.

SCALE_MSH
DOUBLE PRECISION

Scaling factor, applied to the .msh geometry. Note that translation occurs after scaling.

CAD_PROPAGATE_ORDER
CHARACTER

Ray propagation order used to determine whether any point is located inside or outside of the STL surface.

IJK ---------------------------------- Propagation occurs in the I, followed by J, and K directions
JKI ---------------------------------- Propagation occurs in the J, followed by K, and I directions
KIJ ---------------------------------- Propagation occurs in the K, followed by I, and J directions

RAY_DIR
CHARACTER

Ray direction when propagating CAD value

SET_CORNER_CELLS
LOGICAL

Flag to detect and treat corner cells the same way as in the original MFIX version (i.e. without cut cells).

.TRUE. ---------------------------- Some cut cells may be treated as corner cells.
[*.FALSE.*] -------------------------- Do not treat cut cells as corner cells.

FAC_DIM_MAX_CUT_CELL
DOUBLE PRECISION

Factor used to allocate cut cell arrays (expressed as a fraction of DIMENSION_3G).

PG_OPTION
INTEGER

Option for pressure gradient computation in cut cells.

1 ------------------------------------- Use maximum of (east/west), (north/south), and (top/bottom) pairs of velocity cells.
2 ------------------------------------- Use both (east/west), (north/south), and (top/bottom) areas of velocity cells.
[*0*] ------------------------------------ Use east, north and top areas of pressure cell (same as standard cells).

CG_SAFE_MODE
INTEGER

Run code in safe mode.

1 ------------------------------------- Performs initial preprocessing but use all original MFIX subroutines during flow solution (using only cell volumes and areas of cut cells).
[*0*] ------------------------------------ Runs the code with modified subroutines for cut cell treatment.

PRINT_WARNINGS
LOGICAL

Prints any warning message encountered during pre-processing on the screen.

CG_UR_FAC
DOUBLE PRECISION

Under-relaxation factor used in cut cells (only CG_UR_FAC(2) is used).

PRINT_PROGRESS_BAR
LOGICAL

Print a progress bar during each major step of pre-processing stage.

BAR_WIDTH
INTEGER

Width of the progress bar (complete status), expressed in number of characters (between 10 and 80).

BAR_CHAR
CHARACTER

Character used to create the progress bar.

BAR_RESOLUTION
DOUBLE PRECISION

Update frequency of progress bar, expressed in percent of total length (between 1.0 and 100.0).

WRITE_DASHBOARD
LOGICAL

Writes the file dashboard.txt at regular intervals. The file shows a summary of the simulation progress.

F_DASHBOARD
INTEGER

Frequency, expressed in terms of iterations, at which the dashboard is updated.

RE_INDEXING
LOGICAL

Turns on the re-indexing of cells. When true, inactive (dead) cells are removed from computational domain.

ADJUST_PROC_DOMAIN_SIZE
LOGICAL

Attempts to adjust grid partition. Each processor will be assigned its own size to minimize load imbalance.

REPORT_BEST_DOMAIN_SIZE
LOGICAL

Attempts to adjust grid partition. Each processor will be assigned its own size to minimize load imbalance.

NODESI_REPORT
INTEGER

Temporary setting used in serial run to report best domain size for parallel run.

NODESJ_REPORT
INTEGER

Temporary setting used in serial run to report best domain size for parallel run.

NODESK_REPORT
INTEGER

Temporary setting used in serial run to report best domain size for parallel run.

MINIMIZE_SEND_RECV LOGICAL

Attempts to minimize the size of the send/receive layers.

DWALL_BRUTE_FORCE LOGICAL

Brute force calculation of wall distance.

8.5 Gas Phase

This section lists keywords for specifying the gas phase.

RO_G0 DOUBLE PRECISION

Specified constant gas density [g/cm^3 in CGS]. An equation of state -the ideal gas law by default- is used to calculate the gas density if this parameter is undefined. The value may be set to zero to make the drag zero and to simulate granular flow in a vacuum. For this case, users may turn off solving for gas momentum equations to accelerate convergence.

MU_G0 DOUBLE PRECISION

Specified constant gas viscosity [g/(cm.s) in CGS].

K_G0 DOUBLE PRECISION

Specified constant gas conductivity [cal/(s.cm.K) in CGS].

C_PG0 DOUBLE PRECISION

Specified constant gas specific heat [cal/(g.s.K) in CGS].

DIF_G0 DOUBLE PRECISION

Specified constant gas diffusivity [(cm^2/s) in CGS].

MW_AVG DOUBLE PRECISION

Average molecular weight of gas [(g/mol) in CGS]. Used in calculating the gas density for non-reacting flows when the gas composition is not defined.

MW_G(Species) DOUBLE PRECISION

Molecular weight of gas species [(g/mol) in GCS].

NMAX_G INTEGER

Number of species comprising the gas phase.

SPECIES_G(Species) CHARACTER

Name of gas phase species as it appears in the materials database.

SPECIES_ALIAS_G(Species) CHARACTER

User defined name for gas phase species. Aliases are used in specifying chemical equations and must be unique.

8.6 Solids Phase

This section contains keywords for specifying solids phases. Keywords under this section are applicable to all solids models (TFM, DEM, and PIC) unless otherwise stated. Keywords specific to one or more solids models are indicated by the subheadings.

SOLIDS_MODEL(Phase)

CHARACTER

Defines the model used for the solids phase. For TFM/DEM hybrid simulations, first define all TFM solids, then define the DEM solids phases.

TFM	-------------------------------- Two-fluid Model (continuum)
DEM	-------------------------------- Discrete Element Model
PIC	--------------------------------- Multiphase-Particle in Cell

MMAX

INTEGER

Number of solids phases.

Applies to solids models: TFM, DEM, PIC

D_P0(Phase)

DOUBLE PRECISION

Initial particle diameters [cm in CGS].

Applies to solids models: TFM, DEM, PIC

RO_S0(Phase)

DOUBLE PRECISION

Specified constant solids density [g/cm^3 in CGS]. Reacting flows may use variable solids density by leaving this parameter undefined and specifying X_S0 and RO_XS0 as well as the index of the inert species.

Applies to solids models: TFM, DEM, PIC

X_S0(Phase, Species)

DOUBLE PRECISION

Baseline species mass fraction. Specifically, the mass fraction of an unreacted sample (e.g., proximate analysis).

Applies to solids models: TFM, DEM

RO_XS0(Phase, Species)

DOUBLE PRECISION

Specified constant solids species density [g/cm^3 in CGS].

Applies to solids models: TFM, DEM

INERT_SPECIES(Phase, Species)

INTEGER

Index of inert solids phase species. This species should not be a product or reactant of any chemical reaction.

Applies to solids models: TFM, DEM

DIL_INERT_X_VSD(Phase)

DOUBLE PRECISION

Mass fraction of inert solids phase species in the dilute region. In dilute region (see DIL_FACTOR_VSD), the solids density is computed based on this inert species mass fraction, rather than the current inert species mass fraction. This may help convergence when the Variable Solids Density model is invoked.

Applies to solids models: TFM, DEM

DIL_FACTOR_VSD(Phase) DOUBLE PRECISION

Factor to define the dilute region where the solids density is set using DIL_INERT_X_VSD. Cells where the solids volume fraction is between DIL_EP_S and DIL_EP_S x DIL_FACTOR_VSD will automatically set the solids density using DIL_INERT_X_VSD instead of the current inerts species mass fraction. Set this factor to zero to always use the current inert species mass fraction.

Applies to solids models: TFM, DEM

K_S0(Phase) DOUBLE PRECISION

Specified constant solids conductivity [cal/(s.cm.K) in CGS].

Applies to solids models: TFM, DEM

C_PS0(Phase) DOUBLE PRECISION

Specified constant solids specific heat [cal/(g.s.K) in CGS].

Applies to solids models: TFM, DEM

MW_S(Phase, Species) DOUBLE PRECISION

Molecular weight of solids phase species [(g/mol) in CGS].

Applies to solids models: TFM, DEM

NMAX_S(Phase) INTEGER

Number of species comprising the solids phase.

Applies to solids models: TFM, DEM

SPECIES_S(Phase, Species) CHARACTER

Name of solids phase M, species N as it appears in the materials database.

Applies to solids models: TFM, DEM

SPECIES_ALIAS_S(Phase, Species) CHARACTER

User defined name for solids phase species. Aliases are used in specifying chemical equations and must be unique.

Applies to solids models: TFM, DEM

8.6.1 Two Fluid Model (TFM)

Keywords specific to the two fluid model, MFIX-TFM, are defined in this section.

KT_TYPE CHARACTER

Solids phase stress model [LUN_1984]. This is only needed when solving the granular energy PDE (GRANULAR_ENERGY = .TRUE.).

Applies to solids models: TFM

AHMADI	Cao and Ahmadi (1995). Int. J. Multiphase Flow 21(6), 1203.
GD_99	Garzo and Dufty (1999). Phys. Rev. E 59(5), 5895.
GHD	Garzo, Hrenya and Dufty (2007). Phys. Rev. E 76(3), 31304
GTSH	Garzo, Tenneti, Subramaniam, Hrenya (2012). J.Fluid Mech. 712, 129.
IA_NONEP	Iddir & Arastoopour (2005). AIChE J. 51(6), 1620
LUN_1984	Lun et al (1984). J. Fluid Mech., 140, 223.
SIMONIN	Simonin (1996). VKI Lecture Series, 1996-2

FRICTION

LOGICAL

Solids stress model selection.

Applies to solids models: TFM

[*.FALSE.*] -------------------------- Do not use the Princeton solids stress model.

.TRUE. ----------------------------- Use the Princeton solids stress model

SAVAGE

INTEGER

For a term appearing in the frictional stress model invoked with FRICTION keyword.

Applies to solids models: TFM

0 ------------------------------------- Use S:S in the frictional stress model.

[*1*] ------------------------------------ Use an alternate form suggested by Savage.

2 ------------------------------------- An appropriate combination of above.

SCHAEFFER

LOGICAL

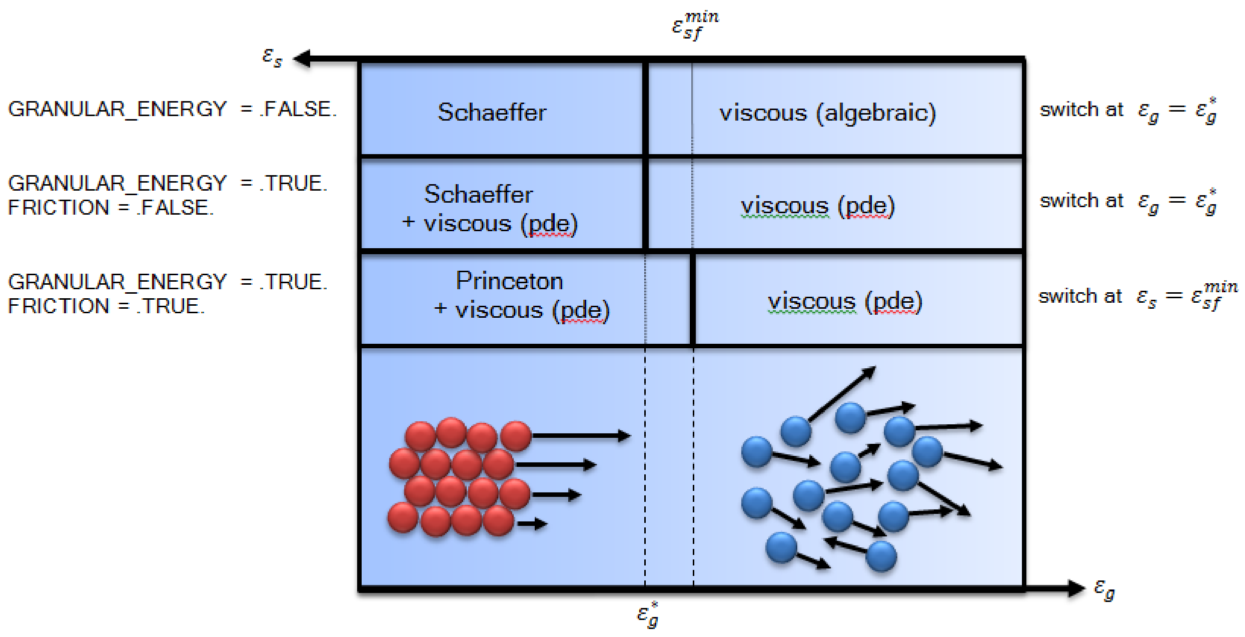
Schaeffer frictional stress tensor formulation.

Applies to solids models: TFM

[*.TRUE.*] ---------------------------- Use the Schaeffer model.

.FALSE. ---------------------------- Do not use the Schaeffer model.

The combination of the keywords GRANULAR_ENERGY and FRICTION invokes different solids stress modes as shown below. Note the dependencies on the other keywords EP_STAR, ε_g^*, and EPS_F_MIN, ε_{sf}^{min}.


ε_{sf}^{min}
ε_s
GRANULAR_ENERGY = .FALSE.
Schaeffer
viscous (algebraic)
switch at $\varepsilon_g = \varepsilon_g^*$
GRANULAR_ENERGY = .TRUE.
FRICTION = .FALSE.
Schaeffer + viscous (pde)
viscous (pde)
switch at $\varepsilon_g = \varepsilon_g^*$
GRANULAR_ENERGY = .TRUE.
FRICTION = .TRUE.
Princeton + viscous (pde)
viscous (pde)
switch at $\varepsilon_s = \varepsilon_{sf}^{min}$
ε_g
ε_g^*

BLENDING_STRESS

LOGICAL

Blend the Schaeffer stresses with the stresses resulting from algebraic kinetic theory around the value of EP_STAR.

Applies to solids models: TFM

TANH_BLEND

LOGICAL

Hyperbolic tangent function for blending frictional stress models.

SIGM_BLEND

LOGICAL

A scaled and truncated sigmoidal function for blending frictional stress models.

Applies to solids models: TFM

YU_STANDISH

LOGICAL

Correlation to compute maximum packing for polydisperse systems.

Applies to solids models: TFM

.TRUE. -----------------------------	Use the Yu and Standish correlation.
[*.FALSE.*] --------------------------	Do not use the Yu and Standish correlation.

FEDORS_LANDEL

LOGICAL

Correlation to compute maximum packing for binary (only) mixtures of powders.

Applies to solids models: TFM

.TRUE. -----------------------------	Use the Fedors and Landel correlation.
[*.FALSE.*] --------------------------	Do not use the Fedors and Landel correlation.

RDF_TYPE

CHARACTER

Radial distribution function at contact for polydisperse systems. Do not specify any RDF for monodisperse systems because Carnahan- Starling is the model only available. Carnahan, N.F. and Starling K.E., (1969). The Journal of Chemical Physics, Vol. 51(2):635-636.

Applies to solids models: TFM

LEBOWITZ ------------------------	Lebowitz, J.L. (1964) The Physical Review, A133, 895-899
MODIFIED_LEBOWITZ --------	Iddir, H. Y., Modeling of the multiphase mixture of particles using the kinetic theory approach. Doctoral Dissertation, Illinois Institute of Technology, Chicago, Illinois, 2004, (chapter 2, equations 2-49 through 2-52.)
MANSOORI -----------------------	Mansoori, GA, Carnahan N.F., Starling, K.E. Leland, T.W. (1971). The Journal of Chemical Physics, Vol. 54:1523-1525.
MODIFIED_MANSOORI -------	van Wachem, B.G.M., Schouten, J.C., van den Bleek, C.M., Krishna, R. and Sinclair, J. L. (2001) AIChE Journal 47:1035&#8211;1051.

ADDED_MASS

LOGICAL

Flag to include the added (or virtual) mass force. This force acts to increase the inertia of the dispersed phase, which tends to stabilize simulations of bubbly gas-liquid flows.

Applies to solids models: TFM

M_AM

INTEGER

The disperse phase number to which the added mass is applied.

Applies to solids models: TFM

C_E

DOUBLE PRECISION

Coefficient of restitution for particle-particle collisions.

Applies to solids models: TFM

R_P(Phase, Phase)
DOUBLE PRECISION

Coefficient of restitution for particle-particle collisions specific to GHD theory implementation.

E_W
DOUBLE PRECISION

Coefficient of restitution for particle-wall collisions when using Johnson and Jackson partial slip BC (BC_JJ_PS).

PHIP
DOUBLE PRECISION

Specularity coefficient associated with particle-wall collisions when using Johnson and Jackson partial slip BC (BC_JJ_PS). If Jenkins small frictional BC are invoked (JENKINS) then phip is not used.

Applies to solids models: TFM

PHIP0
DOUBLE PRECISION

Specify the value of specularity coefficient when the normalized slip velocity goes to zero when BC_JJ_M is .TRUE.. This variable is calculated internally in the code. Do not modify unless an accurate number is known.

Applies to solids models: TFM

C_F
DOUBLE PRECISION

Coefficient of friction between the particles of two solids phases.

Applies to solids models: TFM

PHI
DOUBLE PRECISION

Angle of internal friction (in degrees). Set this value to zero to turn off plastic regime stress calculations.

Applies to solids models: TFM

PHI_W
DOUBLE PRECISION

Angle of internal friction (in degrees) at walls. Set this value to non-zero (PHI_W = 11.31 means TAN_PHI_W = MU = 0.2) when using Johnson and Jackson partial slip BC (BC_JJ_PS) with Friction model or Jenkins small frictional boundary condition.

Applies to solids models: TFM

EPS_F_MIN
DOUBLE PRECISION

Minimum solids fraction above which friction sets in. [0.5] (when FRICTION = .TRUE.)

Applies to solids models: TFM

EP_S_MAX(Phase)
DOUBLE PRECISION

Maximum solids volume fraction at packing for polydisperse systems (more than one solids phase used). The value of EP_STAR may change during the computation if solids phases with different particle diameters are specified and Yu_Standish or Fedors_Landel correlations are used.

Applies to solids models: TFM

SEGREGATION_SLOPE_COEFFICIENT
DOUBLE PRECISION

Used in calculating the initial slope of segregation: see Gera et al. (2004) - recommended value 0.3. Increasing this coefficient results in decrease in segregation of particles in binary mixtures.

Applies to solids models: TFM

V_EX DOUBLE PRECISION

Excluded volume in Boyle-Massoudi stress.

Applies to solids models: TFM

0.0 ---------------------------------- b-m stress is turned off.

MU_S0(Phase) DOUBLE PRECISION

Specified constant viscosity. If any value is specified then: 1) kinetic theory calculations (granular_energy) are off, which means zero granular pressure contribution (P_S = 0), 2) frictional/plastic calculations are off, which means zero frictional viscosity contributions, however, a plastic pressure term is still invoked (P_STAR), and 3) LAMBDA_S = -2/3 MU_S0.

Applies to solids models: TFM

DIF_S0 DOUBLE PRECISION

Specified constant solids diffusivity [(cm^2)/s in CGS].

Applies to solids models: TFM

EP_STAR DOUBLE PRECISION

Packed bed void fraction. Used to calculate plastic stresses (for contribution to viscosity) and when to implement plastic pressure, P_STAR. Specifically, if EP_G < EP_STAR, then plastic pressure is employed in the momentum equations.

Applies to solids models: TFM

CLOSE_PACKED(Phase) LOGICAL

Flag to enable/disable a phase from forming a packed bed. Effectively removes plastic pressure term from the solids phase momentum equation.

Applies to solids models: TFM

[*.TRUE.*] ---------------------------- The phase forms a packed bed with void fraction EP_STAR.

.FALSE. ---------------------------- The phase can exceed close pack conditions so that it maybe behave like a liquid.

JENKINS LOGICAL

This flag effects how the momentum and granular energy boundary conditions are implemented when using BC_JJ_PS BC.

[*.FALSE.*] -------------------------- Use standard boundary conditions.

.TRUE. ---------------------------- Use Jenkins small frictional boundary condition.

8.6.2 Discrete Element Simulations

This subsection contains keywords available to MFIX discrete element simulations using either DEM or PIC solids unless stated otherwise.

The keywords **DISCRETE_ELEMENT** and **MPPIC** are no longer used. Each solids phase model is specified through the **SOLIDS_MODEL** keyword.

PARTICLES
INTEGER

Number of particles to be read in from the particle_input.dat file. This value is overwritten when using automatic particle generation. A simulation with a mass inflow BC can start without solids by setting PARTICLES = 0.

Applies to solids models: DEM, PIC

GENER_PART_CONFIG
LOGICAL

Automatically generate the initial particle position and velocity data based on the parameters specified for each initial condition (IC) region.

Applies to solids models: DEM, PIC

.TRUE.	Generate particle configuration based on the initial condition parameters. Data provided in the particle_input.dat file, if present, is ignored.
[*.FALSE.*]	Particle position and velocity data are provided in the particle_input.dat file. A runtime error occurs if this file is not provided.

DES_ONEWAY_COUPLED
LOGICAL

Run one-way coupled simulations. The fluid does not see the particles in terms of drag force. The effect of particle volume is still felt by the fluid through non-unity voidage values.

Applies to solids models: DEM, PIC

DES_INTG_METHOD
CHARACTER

Time stepping scheme.

Applies to solids models: DEM

EULER	First-Order Euler Scheme.
ADAMS BASHFORTH	Second order ADAMS BASHFORTH scheme (DEM only)

DES_USR_VAR_SIZE
INTEGER

Defines the size of the particle-based user variable: DES_USR_VAR(SIZE, PARTICLES). Information in this array follows the particle throughout a simulation.

Applies to solids models: DEM

DESGRIDSEARCH_IMAX
INTEGER

Number of des grid cells in the I-direction. If left undefined, then it is set by MFIX such that its size equals three times the maximum particle diameter with a minimum of 1 cell.

Applies to solids models: DEM, PIC

DESGRIDSEARCH_JMAX
INTEGER

Number of des grid cells in the J-direction. If left undefined, then it is set by MFIX such that its size equals three times the maximum particle diameter with a minimum of 1 cell.

Applies to solids models: DEM, PIC

DESGRIDSEARCH_KMAX
INTEGER

Number of des grid cells in the K-direction. If left undefined, then it is set by MFIX such that its size equals three times the maximum particle diameter with a minimum of 1 cell.

Applies to solids models: DEM, PIC

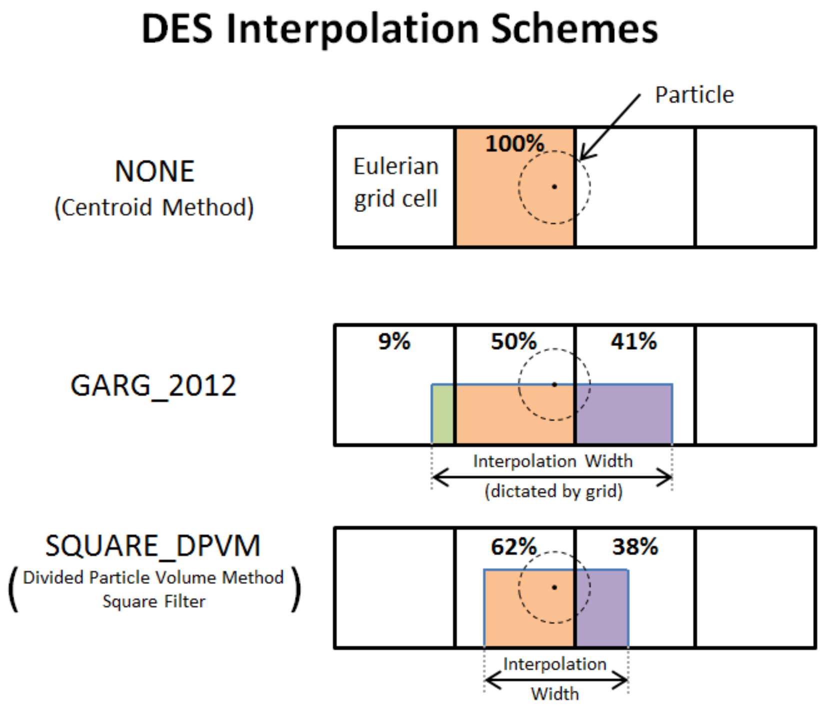
DES_INTERP_SCHEME

CHARACTER

Specify the scheme used to map data to/from a particle's position and the Eulerian grid. This keyword is required when DES_INTERP_MEAN_FIELDS and/or DES_INTERP_ON are specified. A graphical representation of the schemes is shown below.

Applies to solids models: DEM, PIC

NONE -------------------------------	Do not use interpolation.
GARG_2012 ---------------------	Interpolate to/from a particle
SQUARE_DPVM ---------------	Divided Particle Volume Method: Information is interpolated to/from a particles position using a square filter of size DES_INTERP_WIDTH.
LINEAR_HAT --------------------	Linear interpolation: Hat funtions are used to distribute particle information.



DES_INTERP_WIDTH

DOUBLE PRECISION

The length used in interpolating data to/from a particle's position and the Eulerian grid. The interpolation width is only applicable to the DPVM_SQUARE and DPVM_GAUSS interpolation schemes as the GARG_2012 scheme's interpolation width is determined by the Eulerian grid dimensions.

- The interpolation half-width cannot exceed the minimum cell dimension because interpolation is restricted to the 27-cell neighborhood surrounding a particle (9-cell neighborhood in 2D).
- It is recommend that the DES_INTERP_WIDTH be set equal to the maximum particle diameter when using STL defined boundaries. Field data can be smooth by specifying DES_DIFFUSE_WIDTH.

Applies to solids models: DEM

DES_INTERP_ON

LOGICAL

Enables/Disables interpolation of field quantities to a particle's position. This is used in calculating gas-particle interactions, such as the drag force.

Applies to solids models: DEM, PIC

[.*FALSE*.] -------------------------- Use fluid values from the cell containing the particle
.*TRUE*. ---------------------------- Interpolate fluid values from the 27-cell neighborhood to a particle

DES_INTERP_MEAN_FIELDS

LOGICAL

Enables/Disables interpolation of particle data (e.g., solids volume and drag force) from a particle's position to the Eulerian grid.

Applies to solids models: DEM, PIC

[.*FALSE*.] -------------------------- Assign particle data to the fluid grid cell containing the particle
.*TRUE*. ---------------------------- Interpolate particle data from the particle

DES_DIFFUSE_WIDTH

DOUBLE PRECISION

The length scale used to smooth dispersed phase averaged fields by solving a diffusion equation. This approach is typically used when particle sizes near or exceed the size of the Eulerian grid cell sizes.

- Mean filed diffusion is disabled if DES_DIFFUSE_WIDTH is not specified.
- Mean filed diffusion cannot be used with the GARG_2012 interpolation scheme.
- It is recommend that mean field diffusion be used in conjunction with DES_EXPLICITLY_COUPLED to minimize the computational cost of diffusing field data.
- The DES diffusion equation is listed as equation type 10 in the Numerical Parameters section.

Applies to solids models: DEM

DES_EXPLICITLY_COUPLED

LOGICAL

Enable/Disable explicit coupling of DEM solids and the fluid. This algorithm is presently limited to hydrodynamic simulations.

Applies to solids models: DEM

[.*FALSE*.] -------------------------- The fluid and particles calculate interphase forces at their respective time scales. The fluid phase calculates the interphase coupling forces once per fluid time step. Similarly, DEM particles calculate the interface coupling forces at each solids time-step. The DEM must also bin particles to the fluid grid and recalculate the fluid volume fraction every time-step.

.*TRUE*. ---------------------------- Interphase forces are calculated during the fluid time step and stored for each particle. The interphase forces are then distributed among the solids time-steps. This approach can substantially reduce the computational overhead for coupled simulations.

8.6.2.1 Discrete Element Model (DEM)

Keywords specific to the discrete element model, MFIX-DEM, are provided in this section.

NFACTOR

INTEGER

The number of iterations of a pure granular simulation to let the initial particle configuration settle before a coupled gas-solid is started.

NEIGHBOR_SEARCH_N

INTEGER

Maximum number of steps through a DEM loop before a neighbor search will be performed. The search may be called earlier based on other logic.

DES_NEIGHBOR_SEARCH

INTEGER

Flag to set the neighbor search algorithm.

1	N-Square search algorithm (most expensive)
[*4*]	Grid-Based Neighbor Search (Recommended)

NEIGHBOR_SEARCH_RAD_RATIO

DOUBLE PRECISION

Ratio of the distance (imaginary sphere radius) to particle radius that is allowed before a neighbor search is performed. This works in conjunction with the logic imposed by NEIGHBOR_SEARCH_N in deciding calls to the neighbor search algorithm.

FACTOR_RLM

DOUBLE PRECISION

Effectively increase the radius of a particle (multiple of the sum of particle radii) during the building of particle neighbor list.

USE_VDH_DEM_MODEL

LOGICAL

Flag to use van der Hoef et al. (2006) model for adjusting the rotation of the contact plane. See the MFIX-DEM documentation.

DES_COLL_MODEL

CHARACTER

Collision model for the soft-sphere approach used in DEM model. All models require specifying the following parameters: DES_EN_INPUT, DES_EN_WALL_INPUT, MEW, and MEW_W.

LSD	The linear spring-dashpot model. Requires: KN, KN_W, KT_FAC, KT_W_FAC, DES_ETAT_FAC, DES_ETAT_W_FAC.
HERTZIAN	The Hertzian model. Requires: DES_ET_INPUT, DES_ET_WALL_INPUT, E_YOUNG, EW_YOUNG V_POISSON, VW_POISSON.

KN

DOUBLE PRECISION

Normal spring constant [dyne/cm in CGS] for inter-particle collisions. Required when using the linear spring-dashpot collision model.

Applies to solids models: DEM

KT_FAC

DOUBLE PRECISION

Ratio of the tangential spring constant to normal spring constant for inter-particle collisions. Use it to specify the tangential spring constant for particle-particle collisions as KT_FAC*KN. Required when using the linear spring-dashpot collision model.

Applies to solids models: DEM

KN_W

DOUBLE PRECISION

Normal spring constant [dyne/cm in CGS] for particle-wall collisions. Required when using the linear spring-dashpot collision model.

KT_W_FAC

DOUBLE PRECISION

Ratio of the tangential spring constant to normal spring constant for particle-wall collisions. Use it to specify the tangential spring constant for particle-wall collisions as KT_W_FAC*KN_W. Required when using the linear spring-dashpot collision model.

Applies to solids models: DEM

MEW
DOUBLE PRECISION

Inter-particle Coulomb friction coefficient.

Applies to solids models: DEM

MEW_W
DOUBLE PRECISION

Particle-wall Coulomb friction coefficient.

DES_EN_INPUT
DOUBLE PRECISION

The normal restitution coefficient for inter-particle collisions used to determine the inter-particle normal damping factor. Values should be defined for a single dimensional array. For example, a simulation with three solids phases (MMAX=3) needs six values: en11, en12, en13; en22 en 23; en33.

Applies to solids models: DEM

DES_EN_WALL_INPUT
DOUBLE PRECISION

The normal restitution coefficient for particle-wall collisions used to determine the particle-wall normal damping factor. Values should be defined in a single dimensional array. For example, a simulation with three solids phases (MMAX=3) needs three values: enw1, enw2, enw3.

Applies to solids models: DEM

DES_ET_INPUT
DOUBLE PRECISION

Tangential restitution coefficient for inter-particle collisions. Values are defined in a one dimensional array. This is required input when using the Hertzian collision model.

Applies to solids models: DEM

DES_ET_WALL_INPUT
DOUBLE PRECISION

Tangential restitution coefficient for particle wall collisions. Values are defined in a one dimensional array. This is required input when using the Hertzian collision model.

Applies to solids models: DEM

DES_ETAT_FAC
DOUBLE PRECISION

Ratio of the tangential damping factor to the normal damping factor for inter-particle collisions. Required for the linear spring- dashpot model collision model

Applies to solids models: DEM

[*UNDEFINED*] -------------------- For LSD model, if left undefined, MFIX reverts to default value of 0.5

DES_ETAT_W_FAC
DOUBLE PRECISION

Ratio of the tangential damping factor to the normal damping factor for particle-wall collisions. Required for the linear spring-dashpot model for soft-spring collision modelling under DEM. For the Hertzian model, the tangential damping coefficients have to be explicitly specified and specification of this variable is not required.

[*UNDEFINED*] -------------------- For LSD model, if left undefined, MFIX will revert to default value of 0.5

EW_YOUNG
DOUBLE PRECISION

Youngs modulus for the wall [barye in CGS]. Required when using the Hertzian spring-dashpot model.

VW_POISSON
DOUBLE PRECISION

Poisson ratio for the wall. Required when using the Hertzian spring-dashpot model.

E_YOUNG(Phase)
DOUBLE PRECISION

Youngs modulus for the particle [barye in CGS]. Required when using the Hertzian spring-dashpot model.

V_POISSON(Phase)
DOUBLE PRECISION

Poissons ratio for the particle. Required when using the Hertzian spring-dashpot model.

USE_COHESION
LOGICAL

Flag to enable/disable cohesion model.

VAN_DER_WAALS
LOGICAL

Flag to turn on the use Hamaker van der Waals forces.

HAMAKER_CONSTANT
DOUBLE PRECISION

Hamaker constant used in particle-particle cohesive interactions.

WALL_HAMAKER_CONSTANT
DOUBLE PRECISION

Hamaker constant used in particle-wall cohesive interactions.

VDW_OUTER_CUTOFF
DOUBLE PRECISION

Maximum separation distance above which van der Waals forces are not implemented.

VDW_INNER_CUTOFF
DOUBLE PRECISION

Minimum separation distance below which van der Waals forces are calculated using a surface adhesion model.

WALL_VDW_OUTER_CUTOFF
DOUBLE PRECISION

Maximum separation distance above which van der Waals forces are not implemented (particle-wall interactions).

WALL_VDW_INNER_CUTOFF
DOUBLE PRECISION

Minimum separation distance below which van der Waals forces are calculated using a surface adhesion model (particle-wall interactions).

ASPERITIES
DOUBLE PRECISION

Mean radius of surface asperities that influence the cohesive force following a model. See H. Rumpf, Particle Technology, Chapman & Hall, London/New York, 1990.

DES_CONV_CORR
CHARACTER

Specify the Nusselt number correlation used for particle-gas convection.

RANZ_1952	----------------------- Ranz, W.E. and Marshall, W.R. (1952). Chemical Engineering Progress, 48: 141-146 and 173-180

DES_MIN_COND_DIST
DOUBLE PRECISION

Minimum separation distance between the surfaces of two contacting particles.

FLPC DOUBLE PRECISION

Fluid lens proportion constant used to calculate the radius of the fluid lens that surrounds a particle. This parameter is used in the particle-fluid-particle conduction model.

DES_EM(Phase) DOUBLE PRECISION

Emissivity of solids phase M.

E_YOUNG_ACTUAL(Phase) DOUBLE PRECISION

Actual Youngs modulus for the particle [barye in CGS]. Used for computing correction terms for DEM conduction.

EW_YOUNG_ACTUAL(Phase) DOUBLE PRECISION

Actual Youngs modulus for the walls [barye in CGS]. Used for computing correction terms for DEM conduction.

V_POISSON_ACTUAL(Phase) DOUBLE PRECISION

Poissons ratio for the particle. Used for computing correction terms for DEM conduction.

VW_POISSON_ACTUAL DOUBLE PRECISION

Poisson ratio for the wall. Used for computing correction terms for DEM conduction.

MINIMIZE_DES_FACET_LIST LOGICAL

Flag to turn on/off optimizing the list of facets at each des grid cell

8.6.2.2 Particle in Cell (PIC)

Keywords specific to the particle in cell model, MFIX-PIC, are provided in this section. The MFIX-PIC documentation file titled "Documentation of open-source MFIX–PIC software for gas-solids flows" by R. Garg and J. F. Dietiker. This file is located in the mfix-2016.1/doc directory and is available online and serves as the theory guide for the MPPIC model implementation details in MFIX code.

Note that MPPIC model does not work with MPI modules. It has only been tested in serial mode and moderate testing with SMP.

The MPPIC model is invoked when one or more solids phases has the SOLIDS_MODEL set to PIC. There are two methods to specify the initial seeding of parcels. In both methods, the user first defines the physical region where the initial solids will be seeded. This is done by the same flags that are used in continuum representation of dispersed phase. In the first method, the user specifies the number of parcels per cell by the setting the flag "CONSTANTNPC" to TRUE and specifying number of parcels per cell for each phase by the array "NPC_PIC". In this case, the user defined number of parcels per cell is randomly seeded in the initial physical region specified by user. The statistical weight is assigned to parcels such that the solid volume fraction implied by parcels equals the user defined solid volume fraction (see the MPPIC documentation).

In the second method, the statistical weight of parcels is fixed by setting the flag "CONSTANTWT" to TRUE along with specifying the statistical weight of parcels belonging to each phase by the array "STATWT_PIC". The number of parcels per cell is computed by the code such that the solid volume fraction implied by parcels equals the user defined solid volume fraction.

The current implementation of MPPIC model also has the frictional stress model similar to the implementation outlined in "An Incompressible Three-Dimensional Multiphase Particle-in-Cell Model for Dense Particle Flows," by D.M. Snider in the Journal of Computational Physics, volume 170, pages 523-469 (2001). This model does not simulate very stably.
The minimum gas voidage at maximum packing beyond which the MPPIC frictional stress model gets invoked is still defined by the flag EP_STAR that is generally used in continuum representation.

MPPIC_SOLID_STRESS_SNIDER

LOGICAL

Turn on snider's version of frictional model. Does not run very stably.

MPPIC_COEFF_EN1

DOUBLE PRECISION

First coefficient of restitution for the frictional stress model in the MPPIC model. See the MPPIC documentation for more details.

MPPIC_COEFF_EN2

DOUBLE PRECISION

Second coefficient of restitution for the frictional stress model in the MPPIC model. See the MPPIC documentation for more details.

MPPIC_COEFF_EN_WALL

DOUBLE PRECISION

Normal coefficient of restitution for parcel-wall collisions in the MPPIC model.

MPPIC_COEFF_ET_WALL

DOUBLE PRECISION

Tangential coefficient of restitution for parcel-wall collisions in the MPPIC model. Currently not implemented in the code.

MPPIC_PDRAG_IMPLICIT

LOGICAL

Turn on the implicit treatment for interphase drag force. Valid only for MPPIC model.

MPPIC_GRAV_TREATMENT

LOGICAL

Variable to decide if special treatment is needed or not in the direction of gravity in the frictional stress tensor. See the MPPIC documentation for details.

PIC_REPORT_MIN_EPG

LOGICAL

A run time flag to report minimum value and location of gas voidage. This is useful only for debugging and is not recommended for production runs.

PSFAC_FRIC_PIC P_s term in the frictional stress model of Snider.	INTEGER
FRIC_EXP_PIC Beta term in the frictional stress model of Snider.	DOUBLE PRECISION
FRIC_NON_SING_FAC Non-singularity term (epsilon) in the frictional stress model of Snider.	CHARACTER
CFL_PIC CFL number used to decide maximum time step size for parcels evolution equations. Relevant to MPPIC model only.	DOUBLE PRECISION

8.7 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.

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

IC_X_W(IC) X coordinate of the west face.	DOUBLE PRECISION
IC_X_E(IC) X coordinate of the east face.	DOUBLE PRECISION
IC_Y_S(IC) Y coordinate of the south face.	DOUBLE PRECISION
IC_Y_N(IC) Y coordinate of the north face.	DOUBLE PRECISION
IC_Z_B(IC) Z coordinate of the bottom face.	DOUBLE PRECISION

IC_Z_T(IC)
DOUBLE PRECISION

Z coordinate of the top face.

IC_I_W(IC)
INTEGER

I index of the west-most wall.

IC_I_E(IC)
INTEGER

I index of the east-most wall.

IC_J_S(IC)
INTEGER

J index of the south-most wall.

IC_J_N(IC)
INTEGER

J index of the north-most wall.

IC_K_B(IC)
INTEGER

K index of the bottom-most wall.

IC_K_T(IC)
INTEGER

K index of the top-most wall.

IC_TYPE(IC)
CHARACTER

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)
DOUBLE PRECISION

Initial void fraction in the IC region.

IC_P_G(IC)
DOUBLE PRECISION

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)
DOUBLE PRECISION

Initial solids pressure in the IC region. Usually, this value is specified as zero.

IC_L_SCALE(IC)
DOUBLE PRECISION

Turbulence length scale in the IC region.

IC_ROP_S(IC, Phase)
DOUBLE PRECISION

Initial bulk density (rop_s = ro_s x ep_s) of solids phase-m in the IC region. Users need to specify this IC only for polydisperse flow (MMAX > 1). Users must make sure that summation of (IC_ROP_s(ic,m) / RO_s(m)) over all solids phases is equal to (1.0 - IC_EP_g(ic)).

IC_EP_S(IC, Phase) DOUBLE PRECISION

Initial solids volume fraction of solids phase-m in the IC region. This may be specified in place of IC_ROP_s.

IC_T_G(IC) DOUBLE PRECISION

Initial gas phase temperature in the IC region.

IC_T_S(IC, Phase) DOUBLE PRECISION

Initial solids phase-m temperature in the IC region.

IC_THETA_M(IC, Phase) DOUBLE PRECISION

Initial solids phase-m granular temperature in the IC region.

IC_GAMA_RG(IC, Phase) DOUBLE PRECISION

Gas phase radiation coefficient in the IC region. Modify file rdtn2.inc to change the source term.

IC_T_RG(IC, Phase) DOUBLE PRECISION

Gas phase radiation temperature in the IC region.

IC_GAMA_RS(IC, Phase) DOUBLE PRECISION

Solids phase-m radiation coefficient in the IC region. Modify file energy_mod.f to change the source term.

IC_T_RS(IC, Phase) DOUBLE PRECISION

Solids phase-m radiation temperature in the IC region.

IC_U_G(IC) DOUBLE PRECISION

Initial x-component of gas velocity in the IC region.

IC_U_S(IC, Phase) DOUBLE PRECISION

Initial x-component of solids-phase velocity in the IC region.

IC_V_G(IC) DOUBLE PRECISION

Initial y-component of gas velocity in the IC region.

IC_V_S(IC, Phase) DOUBLE PRECISION

Initial y-component of solids-phase velocity in the IC region.

IC_W_G(IC) DOUBLE PRECISION

Initial z-component of gas velocity in the IC region.

IC_W_S(IC, Phase) DOUBLE PRECISION

Initial z-component of solids-phase velocity in the IC region.

IC_X_G(IC, Species) DOUBLE PRECISION

Initial mass fraction of gas species.

IC_X_S(IC, Phase, Species) DOUBLE PRECISION

Initial mass fraction of solids species.

IC_SCALAR(IC, Scalar Eq.) DOUBLE PRECISION

Initial value of Scalar n.

IC_K_TURB_G(IC) DOUBLE PRECISION

Initial value of K in K-Epsilon.

IC_E_TURB_G(IC) DOUBLE PRECISION

Initial value of Epsilon in K-Epsilon.

IC_DES_FIT_TO_REGION(IC) LOGICAL

Flag for inflating initial lattice distribution to the entire IC region.

IC_PIC_CONST_NPC(IC, Phase) INTEGER

Flag to specify the initial constant number of particles per cell for the PIC method initialization. Statistical weight of parcels will be calculated by the code.

IC_PIC_CONST_STATWT(IC, Phase) DOUBLE PRECISION

Flag to specify the initial constant statistical weight for computational particles/parcels. Actual number of parcels will be automatically computed.

8.8 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.

BC_X_W(BC) DOUBLE PRECISION

X coordinate of the west face or edge.

BC_X_E(BC) DOUBLE PRECISION

X coordinate of the east face or edge.

BC_Y_S(BC) DOUBLE PRECISION

Y coordinate of the south face or edge.

BC_Y_N(BC) DOUBLE PRECISION

Y coordinate of the north face or edge.

BC_Z_B(BC) DOUBLE PRECISION

Z coordinate of the bottom face or edge.

BC_Z_T(BC) DOUBLE PRECISION

Z coordinate of the top face or edge.

BC_I_W(BC) INTEGER

I index of the west-most cell.

BC_I_E(BC) INTEGER

I index of the east-most cell.

BC_J_S(BC) INTEGER

J index of the south-most cell.

BC_J_N(BC) INTEGER

J index of the north-most cell.

BC_K_B(BC) INTEGER

K index of the bottom-most cell.

BC_K_T(BC) INTEGER

K index of the top-most cell.

BC_TYPE(BC) CHARACTER

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. Users need to specify all scalar quantities and velocity components. The specified values of fluid and solids velocities are only used initially as MFIX computes these values at this inlet boundary.
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, the Johnson-Jackson boundary condition is used for solids. A FSW is equivalent to using a PSW with hw=0.
NO_SLIP_WALL or *NSW* ------	All components of the velocity vanish at the wall. If BC_JJ_PS is equal to 1, the Johnson-Jackson boundary condition is used for solids. A NSW is equivalent to using a PSW with vw=0 and hw undefined.
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. For free slip set hw = 0. For no slip leave hw undefined (hw=+inf) and set vw = 0. To set hw = +inf, leave it unspecified. If BC_JJ_PS is equal to 1, the Johnson-Jackson boundary condition is used for solids.

8.8.1 Wall boundary conditions

8.8.1.1 Momentum Equations

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. If the Johnson and Jackson partial slip boundary condition is not used (i.e., BC_JJ_PS(bc) = 0), the coefficients hw and vw should be specified. For free slip set hw = 0. For no slip leave hw undefined (hw = ∞) and set vw = 0. To set hw = ∞, leave it unspecified.

BC_HW_G(BC) DOUBLE PRECISION

Gas phase hw for partial slip boundary.

BC_HW_S(BC, Phase) DOUBLE PRECISION

Solids phase hw for partial slip boundary.
.

BC_UW_G(BC) DOUBLE PRECISION

Gas phase Uw for partial slip boundary.

BC_UW_S(BC, Phase) DOUBLE PRECISION

Solids phase Uw for partial slip boundary.

BC_VW_G(BC) DOUBLE PRECISION

Gas phase Vw for partial slip boundary.

BC_VW_S(BC, Phase) DOUBLE PRECISION

Solids phase Vw for partial slip boundary.

BC_WW_G(BC) DOUBLE PRECISION

Gas phase Ww for partial slip boundary.

BC_WW_S(BC, Phase) DOUBLE PRECISION

Solids phase Ww for partial slip boundary.

BC_JJ_PS(BC) INTEGER

Johnson and Jackson partial slip BC.

0 ------------------------------------- Do not use Johnson and Jackson partial slip boundary condition.

1 ------------------------------------- Use Johnson and Jackson partial slip boundary condition.

8.8.1.2 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 the Johnson and Jackson partial slip boundary condition is not used (i.e., BC_JJ_PS(bc) = 0), the coefficients hw and c should be specified. For specified heat flux set hw=0 and give a value for c. For specified temperature boundary condition leave hw unspecified (hw=∞ and give a value for Tw.

BC_THETAW_M(BC, Phase) DOUBLE PRECISION

Specified wall value, THETAw_M, in diffusion boundary condition: d(Theta_M)/dn + Hw (THETA_M - THETAw_M) = C, where n is the fluid-to-wall normal.

BC_HW_THETA_M(BC, Phase) DOUBLE PRECISION

Transfer coefficient, Hw, in diffusion boundary condition: d(Theta_M)/dn + Hw (THETA_M - THETAw_M) = C, where n is the fluid-to-wall normal.

BC_C_THETA_M(BC, Phase) DOUBLE PRECISION

Specified constant flux, C, in diffusion boundary condition: d(Theta_M)/dn + Hw (THETA_M - THETAw_M) = C, where n is the fluid-to-wall normal.

8.8.1.3 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) DOUBLE PRECISION

Gas phase heat transfer coefficient, Hw, in diffusion boundary condition: d(T_g)/dn + Hw (T_g - Tw_g) = C, where n is the fluid-to-wall normal.

BC_TW_G(BC) DOUBLE PRECISION

Specified gas phase wall temperature, Tw_g, in diffusion boundary condition: d(T_g)/dn + Hw (T_g - Tw_g) = C, where n is the fluid-to-wall normal.

BC_C_T_G(BC) DOUBLE PRECISION

Specified constant gas phase heat flux, C, in diffusion boundary condition: d(T_g)/dn + Hw (T_g - Tw_g) = C, where n is the fluid-to-wall normal.

BC_HW_T_S(BC, Phase) DOUBLE PRECISION

Solids phase heat transfer coefficient, Hw, in diffusion boundary condition: d(T_s)/dn + Hw (T_s - Tw_s) = C, where n is the fluid-to-wall normal.

BC_TW_S(BC, Phase) DOUBLE PRECISION

Specified solids phase wall temperature, Tw_s, in diffusion boundary condition: d(T_s)/dn + Hw (T_s - Tw_s) = C, where n is the fluid-to-wall normal.

BC_C_T_S(BC, Phase) DOUBLE PRECISION

Specified constant solids phase heat flux, C, in diffusion boundary condition: d(T_s)/dn + Hw (T_s - Tw_s) = C, where n is the fluid-to-wall normal.

8.8.1.4 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_HW_X_G(BC, Species) DOUBLE PRECISION

Gas phase species mass transfer coefficient, Hw, in diffusion boundary condition: d(X_g)/dn + Hw (X_g - Xw_g) = C, where n is the fluid-to-wall normal.

BC_XW_G(BC, Species) DOUBLE PRECISION

Specified wall gas species mass fraction, Xw, in diffusion boundary condition: d(X_g)/dn + Hw (X_g - Xw_g) = C, where n is the fluid-to-wall normal.

BC_C_X_G(BC, Species) DOUBLE PRECISION

Specified constant gas species mass flux, C, in diffusion boundary condition: d(X_g)/dn + Hw (X_g - Xw_g) = C, where n is the fluid-to-wall normal.

BC_HW_X_S(BC, Phase, Species) DOUBLE PRECISION

Solid phase species mass transfer coefficient, Hw, in diffusion boundary condition: d(X_s)/dn + Hw (X_s - Xw_s) = C, where n is the fluid-to-wall normal.

BC_XW_S(BC, Phase, Species) DOUBLE PRECISION

Specified solids species mass fraction at the wall, Xw, in diffusion boundary condition: d(X_g)/dn + Hw (X_g - Xw_g) = C, where n is the fluid-to-wall normal.

BC_C_X_S(BC, Phase, Species) DOUBLE PRECISION

Specified constant solids species mass flux, C, in diffusion boundary condition: d(X_s)/dn + Hw (X_s - Xw_s) = C, where n is the fluid-to-wall normal.

8.8.1.5 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, Scalar Eq.) DOUBLE PRECISION

Scalar transfer coefficient, Hw, in diffusion boundary condition: d(Scalar)/dn + Hw (Scalar - ScalarW) = C, where n is the fluid-to-wall normal.

BC_SCALARW(BC, Scalar Eq.) DOUBLE PRECISION

Specified scalar value at the wall, ScalarW, in diffusion boundary condition: d(Scalar)/dn + Hw (Scalar - ScalarW) = C, where n is the fluid-to-wall normal.

BC_C_SCALAR(BC, Scalar Eq.) DOUBLE PRECISION

Specified constant scalar flux, C, in diffusion boundary condition: d(Scalar)/dn + Hw (Scalar - ScalarW) = C, where n is the fluid-to-wall normal.

8.8.2 Flow Boundary Conditions

BC_EP_G(BC) DOUBLE PRECISION

Void fraction at the BC plane.
.

BC_P_G(BC) DOUBLE PRECISION

Gas pressure at the BC plane.

BC_ROP_S(BC, Phase) DOUBLE PRECISION

Bulk density of solids phase at the BC plane.

BC_EP_S(BC, Phase) DOUBLE PRECISION

Solids volume fraction at the BC plane.

BC_T_G(BC) DOUBLE PRECISION

Gas phase temperature at the BC plane.

BC_T_S(BC, Phase) DOUBLE PRECISION

Solids phase-m temperature at the BC plane.

BC_THETA_M(BC, Phase) Solids phase-m granular temperature at the BC plane.	DOUBLE PRECISION
BC_X_G(BC, Species) Mass fraction of gas species at the BC plane.	DOUBLE PRECISION
BC_X_S(BC, Phase, Species) Mass fraction of solids phase at the BC plane.	DOUBLE PRECISION
BC_U_G(BC) X-component of gas velocity at the BC plane.	DOUBLE PRECISION
BC_U_S(BC, Phase) X-component of solids-phase velocity at the BC plane.	DOUBLE PRECISION
BC_V_G(BC) Y-component of gas velocity at the BC plane.	DOUBLE PRECISION
BC_V_S(BC, Phase) Y-component of solids-phase velocity at the BC plane.	DOUBLE PRECISION
BC_W_G(BC) Z-component of gas velocity at the BC plane.	DOUBLE PRECISION
BC_W_S(BC, Phase) Z-component of solids-phase velocity at the BC plane.	DOUBLE PRECISION

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.

BC_VOLFLOW_G(BC) DOUBLE PRECISION

Gas volumetric flow rate through the boundary.

.

BC_VOLFLOW_S(BC, Phase) DOUBLE PRECISION

Solids volumetric flow rate through the boundary.

BC_MASSFLOW_G(BC) DOUBLE PRECISION

Gas mass flow rate through the boundary.

BC_MASSFLOW_S(BC, Phase) DOUBLE PRECISION

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.

BC_DT_0(BC) DOUBLE PRECISION

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(BC) DOUBLE PRECISION

Value of normal velocity during the initial interval BC_DT_0.

BC_DT_H(BC) DOUBLE PRECISION

The interval when normal velocity is equal to BC_Jet_gh.

BC_JET_GH(BC) DOUBLE PRECISION

Value of normal velocity during the interval BC_DT_h.

BC_DT_L(BC) DOUBLE PRECISION

The interval when normal velocity is equal to BC_JET_gL.

BC_JET_GL(BC) DOUBLE PRECISION

Value of normal velocity during the interval BC_DT_L.

BC_SCALAR(BC, Scalar Eq.) DOUBLE PRECISION

Boundary value for user-defined scalar equation.

BC_K_TURB_G(BC) DOUBLE PRECISION

Boundary value of K for K-Epsilon Equation.

BC_E_TURB_G(BC) DOUBLE PRECISION

Boundary value of Epsilon for K-Epsilon Equation.

BC_VELMAG_G(BC) DOUBLE PRECISION

Magnitude of gas velocity in a specified boundary region.

BC_VELMAG_S(BC, Phase) DOUBLE PRECISION

Magnitude of gas velocity in a specified boundary region.

BC_PIC_MI_CONST_NPC(BC, Phase) INTEGER

Flag to specify the constant number of computational particles per cell for the PIC solids inflow BC. Statistical weight of parcels will be calculated by the code.

BC_PIC_MI_CONST_STATWT(BC, Phase) DOUBLE PRECISION

Flag to specify the constant statistical weight for inflowing computational particles/parcels. Actual number of parcels will be automatically computed.

BC_PO_APPLY_TO_DES(BC) LOGICAL

Flag to make the PO BC invisible to discrete solids. Set this flag to.FALSE.to remove this BC for discrete solids.

BC_MI_AS_WALL_FOR_DES(BC) LOGICAL

Flag to make the inflow plane invisible to discrete solids. Set this flag to.FALSE.to remove to inflow plane.

BC_JJ_M LOGICAL

Use the modified Johnson and Jackson partial slip BC with variable specularity coefficient.

8.9 Internal Surface

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.

IS_X_W(IS) DOUBLE PRECISION

X coordinate of the west face or edge.

IS_X_E(IS) DOUBLE PRECISION

X coordinate of the east face or edge.

IS_Y_S(IS) DOUBLE PRECISION

Y coordinate of the south face or edge

IS_Y_N(IS) DOUBLE PRECISION

Y coordinate of the north face or edge

IS_Z_B(IS) DOUBLE PRECISION

Z coordinate of the bottom face or edge

IS_Z_T(IS) DOUBLE PRECISION

Z coordinate of the top face or edge

IS_I_W(IS) INTEGER

I index of the west-most cell.

IS_I_E(IS) INTEGER

I index of the east-most cell

IS_J_S(IS) INTEGER

J index of the south-most cell

IS_J_N(IS) INTEGER

J index of the north-most cell

IS_K_B(IS) INTEGER

K index of the bottom-most cell

IS_K_T(IS) INTEGER

K index of the top-most cell

IS_TYPE(IS) CHARACTER

Type of internal surface

IMPERMEABLE or *IP* -----------	No gas or solids flow through the surface.
SEMIPERMEABLE or *SP* -----	Gas flows through the surface with an additional resistance. Solids velocity through the surface is set to zero or to a user- specified fixed value (i.e., solids momentum equation for this direction is not solved).

IS_PC(IS, IDX) DOUBLE PRECISION

Parameters defining the internal surface. 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.

- IDX=1: Permeability [1.E32]
- IDX=2: Inertial resistance coefficient [0.0]

IS_VEL_S(IS, Phase) DOUBLE PRECISION

Value of fixed solids velocity through semipermeable surfaces.

8.10 Point Sources

Point sources (PS) are used in place of mass inlets where either the geometry and/or grid resolution prohibit proper boundary condition specification. For example, a point source may be used to model an injector with dimensions smaller than the grid. Point sources may be defined within a single computational cell, along a plane, or as a volume of computational cells.

Point sources introduce mass directly into a computational cell unlike a boundary condition which specifies flow along a cell face. One consequence of this implementation is that point sources are subjected to convection/diffusion forces and may not travel parallel to the specified directional preference. Directional preference is specified with a velocity vector (i.e., PS_U_g, PS_V_g, etc.), however, directional preference is not required.

Examples showing how to setup point sources can be found in: /mfix-2016.1/tutorials/point_source_spiral

PS_X_W(PS) DOUBLE PRECISION

X coordinate of the west face or edge.
.

PS_X_E(PS) DOUBLE PRECISION

X coordinate of the east face or edge.

PS_Y_S(PS) DOUBLE PRECISION

Y coordinate of the south face or edge.

PS_Y_N(PS) DOUBLE PRECISION

Y coordinate of the north face or edge.

PS_Z_B(PS) DOUBLE PRECISION

Z coordinate of the bottom face or edge.

PS_Z_T(PS) Z coordinate of the top face or edge.	DOUBLE PRECISION
PS_I_W(PS) I index of the west-most cell.	INTEGER
PS_I_E(PS) I index of the east-most cell.	INTEGER
PS_J_S(PS) J index of the south-most cell.	INTEGER
PS_J_N(PS) J index of the north-most cell.	INTEGER
PS_K_B(PS) K index of the bottom-most cell.	INTEGER
PS_K_T(PS) K index of the top-most cell.	INTEGER
PS_U_G(PS) X-component of incoming gas velocity.	DOUBLE PRECISION
PS_V_G(PS) Y-component of incoming gas velocity.	DOUBLE PRECISION
PS_W_G(PS) Z-component of incoming gas velocity.	DOUBLE PRECISION
PS_MASSFLOW_G(PS) Gas mass flow rate through the point source.	DOUBLE PRECISION
PS_T_G(PS) Temperature of incoming gas.	DOUBLE PRECISION
PS_X_G(PS, Species) Gas phase incoming species n mass fraction.	DOUBLE PRECISION
PS_U_S(PS, Phase) X-component of incoming solids velocity.	DOUBLE PRECISION
PS_V_S(PS, Phase) Y-component of incoming solids velocity.	DOUBLE PRECISION

PS_W_S(PS, Phase) DOUBLE PRECISION
Z-component of incoming solids velocity.

PS_MASSFLOW_S(PS, Phase) DOUBLE PRECISION
Solids mass flow rate through the point source.

PS_T_S(PS, Phase) DOUBLE PRECISION
Temperature of incoming solids.

PS_X_S(PS, Phase, Species) DOUBLE PRECISION
Solids phase incoming species n mass fraction.

8.11 Output Control

Keywords for controlling the output are provided in this section.

RES_DT *Required* DOUBLE PRECISION
Interval at which restart (.res) file is updated.

RES_BACKUP_DT DOUBLE PRECISION
Interval at which a backup copy of the restart file is created.

RES_BACKUPS INTEGER
The number of backup restart files to retain.

SPX_DT(SP Value) DOUBLE PRECISION
Interval at which .SPX files are updated.

- SP1: void fraction (EP_G)
- SP2: Gas pressure (P_G) and Solids pressure (P_star)
- SP3: Gas velocity (U_G, V_G, W_G)
- SP4: Solids velocity (U_S, V_S, W_S)
- SP5: Solids bulk density (ROP_s)
- SP6: Gas and solids temperature (T_G, T_S)
- SP7: Gas and solids mass fractions (X_G, X_S)
- SP8: Granular temperature (THETA_M)
- SP9: User defined scalars. (SCALAR)
- SPA: Reaction Rates (ReactionRates)
- SPB: Turbulence quantities (K_TURB_G, E_TURB_G)

NRR INTEGER
The number of user defined chemical reactions stored in the *.SPA file.

OUT_DT

DOUBLE PRECISION

Interval at which standard output (.OUT) file is updated. Only run configuration information is written if left undefined. Otherwise all field variables for the entire domain are written in ASCII format to the .OUT file at OUT_DT intervals.

NLOG

INTEGER

Number of time steps between .LOG file updates.

FULL_LOG

LOGICAL

Display the residuals on the screen and provide messages about convergence on the screen and in the .LOG file.

RESID_STRING(Residual Index)

CHARACTER

Specifies the residuals to display.

P0	Gas pressure
PM	Solids phase M pressure
R0	Gas density
RM	Solids phase M density
U0	Gas phase U-velocity
V0	Gas phase V-velocity
W0	Gas phase W-velocity
UM	Solids phase M U-velocity
VM	Solids phase M V-velocity
WM	Solids phase M W-velocity
T0	Gas temperature
TM	Solids phase M temperature
X0NN	Gas phase species NN mass fraction
XMNN	Solids phase M species NN mass fraction
K0	K-Epsilon model residuals

GROUP_RESID

LOGICAL

Display residuals by equation.

REPORT_NEG_DENSITY

LOGICAL

Provide detailed logging of negative density errors.

[*.FALSE.*]	Do not log negative density errors.
.TRUE.	Log negative density errors.

REPORT_MASS_BALANCE_DT

DOUBLE PRECISION

Frequency to perform an overall species mass balance. Leaving undefined suppresses the mass balance calculations which can slightly extend run time.

PHIP_OUT_JJ

LOGICAL

Output the variable specularity coefficient when BC_JJ_M is .TRUE.. The specularity coefficient will be stored in ReactionRates array for post-processing by post-mfix. User needs to set NRR to 1 for this purpose. Be careful with this setting when reacting flow is simulated.

BDIST_IO

LOGICAL

Use distributed IO :: Each MPI process generates RES/SPx files.

BSTART_WITH_ONE_RES

LOGICAL

Restart a serial IO run (only one RES file was created) with distributed IO.

BWRITE_NETCDF(NetCDF Variable Reference)

LOGICAL

Flag to write variable in NetCDF output file. NetCDF support is not included in MFIX by default. The executable must be compiled and linked with an appropriate NetCDF library to use this functionality. Variable Index List:

- 1: void fraction (EP_G)
- 2: Gas pressure (P_G)
- 3: Solids pressure (P_star)
- 4: Gas velocity (U_G, V_G, W_G)
- 5: Solids velocity (U_S, V_S, W_S)
- 6: Solids bulk density (ROP_s)
- 7: Gas temperature (T_G)
- 8: Gas and solids temperature (T_S)
- 9: Gas mass fractions (X_G)
- 10: Solids mass fractions (X_S)
- 11: Granular temperature (THETA_M)
- 12: User defined scalars. (SCALAR)
- 13: Reaction Rates (ReactionRates)
- 14: Turbulence quantities (K_TURB_G, E_TURB_G)

.TRUE. ---------------------------- Write variable in NetCDF output.

[*.FALSE.*] -------------------------- Do not include variable in NetCDF output.

WRITE_VTK_FILES

LOGICAL

Write VTK files at regular intervals.

[*.FALSE.*] -------------------------- Do not write VTK files. if there are cut cells, they will not be displayed from the usual .res file

.TRUE. ---------------------------- Valid only if Cartesian_grid = .true.

TIME_DEPENDENT_FILENAME

LOGICAL

Use time-dependent VTK file names

.FALSE. --------------------------- The VTK file overwrites the previous file (recommended for steady-state computation).

[*.TRUE.*] --------------------------- A sequential integer is appended to the VTK filenames as they are written to create a series of files (recommended for transient computation).

VTK_DT

DOUBLE PRECISION

Interval (expressed in seconds of simulation time) at which VTK files are written.

VTK_VAR

INTEGER

List of variables written in the VTK files.

1	Void fraction (EP_g)
2	Gas pressure, solids pressure (P_g, P_star)
3	Gas velocity (U_g, V_g, W_g)
4	Solids velocity (U_s, V_s, W_s)
5	Solids density (ROP_s)
6	Gas and solids temperature (T_g, T_s)
7	Gas and solids mass fractions (X_g, X_s)
8	Granular temperature (Theta_m)
9	Scalar
10	Reaction rates
11	K and Epsilon
12	Vorticity magnitude and lambda_2
100	Grid Partition
101	Boundary Condition ID
102	Distance to wall
103	DEM facet count
104	DEM Neighboring facets
999	Cell IJK index
1000	Cut face normal vector

VTK_EP_G

LOGICAL

Write void fraction in VTK file.

VTK_P_G

LOGICAL

Write gas pressure in VTK file.

VTK_P_STAR

LOGICAL

Write solids pressure in VTK file.

VTK_VEL_G

LOGICAL

Write gas velocity vector in VTK file.

VTK_U_G

LOGICAL

Write x-component of gas velocity vector in VTK file.

VTK_V_G

LOGICAL

Write y-component of gas velocity vector in VTK file.

VTK_W_G

LOGICAL

Write z-component of gas velocity vector in VTK file.

VTK_VEL_S

LOGICAL

Write solids velocity vector in VTK file.

VTK_U_S Write x-component of solids velocity vector in VTK file.	LOGICAL
VTK_V_S Write y-component of solids velocity vector in VTK file.	LOGICAL
VTK_W_S Write z-component of solids velocity vector in VTK file.	LOGICAL
VTK_ROP_S Write solids bulk density in VTK file.	LOGICAL
VTK_T_G Write gas temperature in VTK file.	LOGICAL
VTK_T_S Write solids temperature in VTK file.	LOGICAL
VTK_X_G Write gas phase species in VTK file.	LOGICAL
VTK_X_S Write solids phase species in VTK file.	LOGICAL
VTK_THETA_M Write granular temperature in VTK file.	LOGICAL
VTK_SCALAR Write scalar in VTK file.	LOGICAL
VTK_RRATE Write reaction rates in VTK file.	LOGICAL
VTK_K_TURB_G Write turbulent kinetic energy in VTK file.	LOGICAL
VTK_E_TURB_G Write turbulent dissipation rate in VTK file.	LOGICAL
VTK_VORTICITY Write vorticity magnitude in VTK file.	LOGICAL
VTK_LAMBDA_2 Write lambda_2 in VTK file.	LOGICAL

VTK_PARTITION
LOGICAL

Write void grid partition in VTK file.

VTK_BC_ID
LOGICAL

Write boundary condition ID in VTK file.

VTK_DWALL
LOGICAL

Write wall distance in VTK file.

VTK_FACET_COUNT_DES
LOGICAL

Write STL facet count for DES in VTK file.

VTK_NB_FACET_DES
LOGICAL

Write neighboring facets in VTK file.

VTK_IJK
LOGICAL

Write cell IJK index in VTK file.

VTK_NORMAL
LOGICAL

Write cut face normal vector in VTK file.

VTK_DEBUG
LOGICAL

Write debug variable in VTK file.

VTK_DATA
CHARACTER

Type of data to write in the VTK file.

C ------------------------------------- Cell data (VTU file).
P ------------------------------------- Particle data (VTP file).

VTK_SLICE_TOL
DOUBLE PRECISION

Tolerance to detect particle in a VTK region.

VTK_SELECT_MODE
CHARACTER

Particle selection mode in a VTK region.

C ------------------------------------- Select particles with centers inside the VTK region.
P ------------------------------------- Select particles that are entirely inside the VTK region.
I -------------------------------------- Select particles that are inside or intersect the edges of the VTK region.

VTK_PART_DIAMETER
LOGICAL

Write particle radius in VTK file.

VTK_PART_VEL
LOGICAL

Write particle velocity in VTK file.

VTK_PART_ANGULAR_VEL Write particle angular velocity in VTK file.	LOGICAL
VTK_PART_ORIENTATION Write particle angular velocity in VTK file.	LOGICAL
VTK_PART_USR_VAR Write particle user-defined variable in VTK file.	LOGICAL
VTK_PART_TEMP Write particle temperature in VTK file.	LOGICAL
VTK_PART_X_S Write particle species mass fraction in VTK file.	LOGICAL
VTK_PART_COHESION Write particle cohesion in VTK file.	LOGICAL
FRAME Starting Index appended to VTU files	INTEGER
VTU_DIR Directory where vtk files are stored (default is run directory)	CHARACTER
VTK_X_W West location of VTK region.	CHARACTER
VTK_X_E East location of VTK region.	DOUBLE PRECISION
VTK_Y_S South location of VTK region.	CHARACTER
VTK_Y_N North location of VTK region.	DOUBLE PRECISION
VTK_Z_B Bottom location of VTK region.	CHARACTER
VTK_Z_T West location of VTK region.	DOUBLE PRECISION

DES_REPORT_MASS_INTERP LOGICAL

Reports mass based on Lagrangian particles and continuum representation. Useful to ensure mass conservation between Lagrangian and continuum representations. Recommended use for debugging purposes.

Applies to solids models:, DEM, PIC

PRINT_DES_DATA LOGICAL

Allows writing of discrete particle data to output files. Relevant to both granular and coupled simulations.

Applies to solids models:, DEM, PIC

VTP_DIR CHARACTER

Directory where particle vtp files are stored. The files are written in the run directory by default.

DES_OUTPUT_TYPE CHARACTER

The output file format for DES data.

Applies to solids models: DEM, PIC

PARAVIEW	---------------------- ParaView formatted files (.vtp)
TECPLOT	------------------------ Tecplot formatted files (.dat)

DEBUG_DES LOGICAL

Runtime flag to generate debugging information. Additional data for FOCUS_PARTICLE is saved.

Applies to solids models: DEM, PIC

FOCUS_PARTICLE INTEGER

Specify particle number for particle level debugging details.

Applies to solids models: DEM, PIC

PIC_REPORT_SEEDING_STATS LOGICAL

Flag to print processor level parcel seeding statistics for inflow BC with PIC model.

Applies to solids models: PIC

PIC_REPORT_DELETION_STATS LOGICAL

Flag to print processor level parcel deletion statistics for outflow BC with PIC model. Not recommended for production runs.

Applies to solids models: PIC

8.12 User-defined functions

Users may modify any *.f or *.inc file under the MFIX model directory. To modify a file, first copy it from the model directory into the run directory. All modifications should be made to the file in the run directory.

For example, list the contents of the adiabaticFlame test case located in the legacy_tests directory:

```
> cd ~/mfix-2016.1/legacy_tests/adiabaticFlame
> ls
```

```
AUTOTEST  mfix.dat  usr3.f  usr_rates.f
```
The AUTOTEST directory contains data from previous runs and is used for regression testing. The mfix.dat file contains the simulation setup and usr3.f and usr_rates.f contain user-defined functions (UDFs) required by this simulation.

Running **configure_mfix** and setting the computer to the GNU Fortran compiler with O2 optimization with debugging symbols:
```
> ../../configure_mfix FC=gfortran FCFLAGS="-O2 -g"
```
Again, listing the contents of the directory will show the created Makefile
```
> ls
AUTOTEST  Makefile  mfix.dat  usr3.f  usr_rates.f
```
Running **make** to generate the executable
```
> make
Processing chemical reaction data.
Reaction data was successfully processed.
...
```
The first two lines of output indicate that chemical reaction data in the mfix.dat was processed successfully. Listing the files in the directory after compiling:
```
> ls
AUTOTEST  mfix      species.inc  usr3.f usr_rates.d  usr_rates.o
Makefile  mfix.dat  usr3.d       usr3.o usr_rates.f
```
The species.inc file was generated during the reaction preprocessing step. The .d and .o files are intermediate dependency and object files that are created and linked with the executable, mfix.

The following is a list of MFIX files that are usually modified to include user defined scalars, user defined drag models, and chemical reactions, physical properties, and source terms for the governing equations:

File Name:	**Usage Description**
scalar_prop.f	Properties and source terms in scalar transport equations.
usr_drag.f	User-defined drag function.
usr_rates.f	Chemical reaction rates.
usr_rates_des.f[1]	DES chemical reaction rates.
usr_properties.f	Physical properties (density, specific heat, etc.)
usr_sources.f	Governing equation source terms.

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

File Name:	**Usage Description**
write_usr0.f	Called once at the start of a run. This file is typically used for opening user-defined output files.

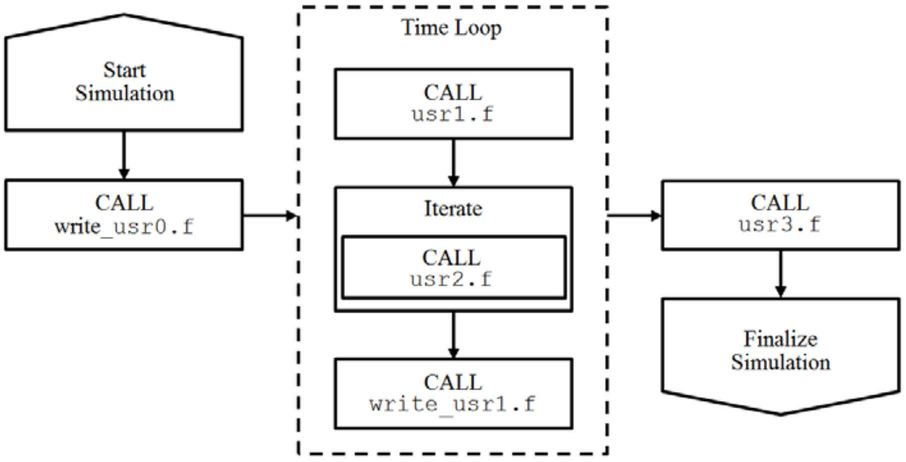
write_usr1.f	Called at intervals defined by USR_DT

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

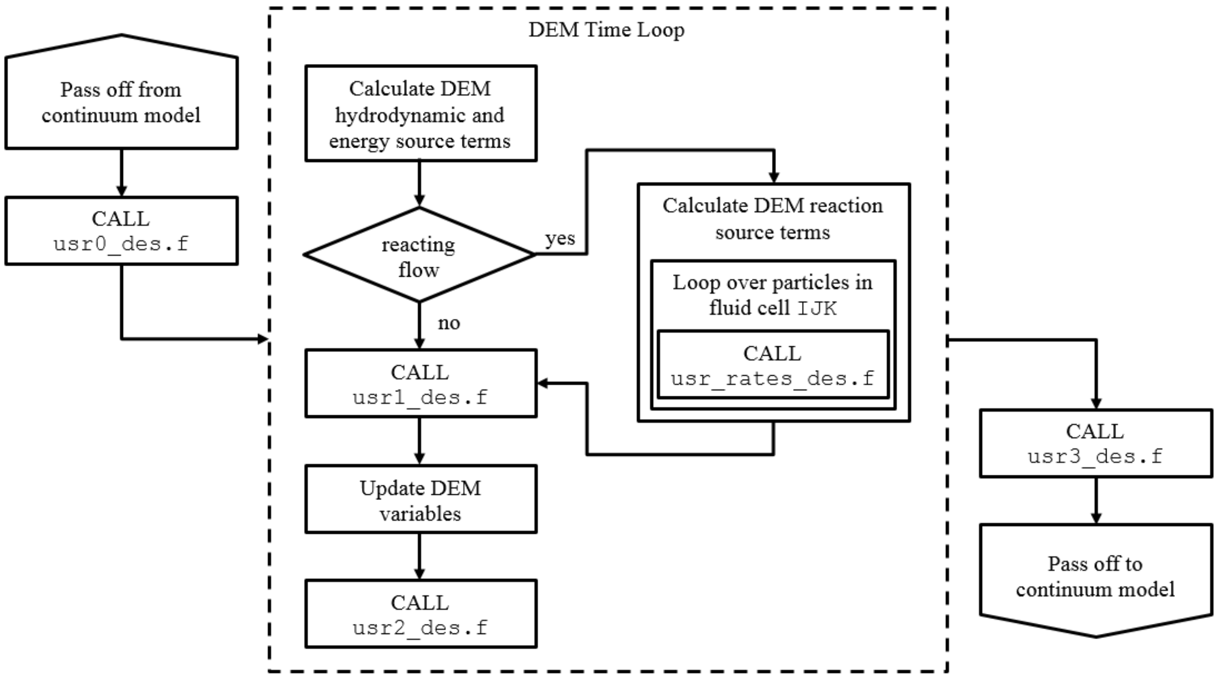
File Name:	**Usage Description**
usr0.f	A subroutine that is called once every run, just before the time-loop begins.
usr1.f	A subroutine that is called once every timestep.
usr2.f	A subroutine that is called once every iteration.
usr3.f	A subroutine that is called once every run, after the time-loop 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.
usr0_des.f[1]	A subroutine called before entering the DES time loop.
usr1_des.f[1]	A subroutine called every DEM timestep after calculating DES source terms but before source terms are applied to the particles.
usr2_des.f[1]	A subroutine called every DES timestep after source terms are applied to the particles.
usr3_des.f[1]	A subroutine that is called after completing the DES time loop.

[1] Denotes files contained in the DES subfolder (mfix-2016.1/model/des/).

User-defined subroutines call structure:



DES User-defined subroutines call structure:


Pass off from continuum model
CALL usr0_des.f
DEM Time Loop
Calculate DEM hydrodynamic and energy source terms
reacting flow
yes
no
Calculate DEM reaction source terms
Loop over particles in fluid cell IJK
CALL usr_rates_des.f
CALL usr1_des.f
Update DEM variables
CALL usr2_des.f
CALL usr3_des.f
Pass off to continuum model

CALL_USR

LOGICAL

Flag to enable user-defined subroutines: USR0, USR1, USR2, USR3, USR0_DES, USR1_DES, USR2_DES, USR3_DES, USR4_DES.

.TRUE. ---------------------------- Call user-defined subroutines.

[*.FALSE.*] -------------------------- Do NOT call user-defined subroutines.

CALL_USR_SOURCE(Equation ID Number)

LOGICAL

Flag to enable user_defined subroutine, usr_source, for calculating source terms in the indicated equation.

.TRUE. ---------------------------- Call user-defined source.

[*.FALSE.*] -------------------------- MFIX default: No additional source.

USR_ROG

LOGICAL

Flag to use the User Defined Function, USR_PROP_ROg, in model/usr_prop.f for calculating the gas phase density, RO_g.

.TRUE. ---------------------------- Call user-defined function.

[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_CPG

LOGICAL

Flag to use the User Defined Function, USR_PROP_CPg, in model/usr_prop.f for calculating the gas phase constant pressure specific heat, C_pg.

.TRUE. ---------------------------- Call user-defined function.

[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_KG

LOGICAL

Flag to use the User Defined Function, USR_PROP_Kg, in model/usr_prop.f for calculating the gas phase conductivity, K_g.

.TRUE. ---------------------------- Call user-defined function.

[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_DIFG

LOGICAL

Flag to use the User Defined Function, USR_PROP_Difg, in model/usr_prop.f for calculating the gas phase diffusivity, Dif_g.

.TRUE. ---------------------------- Call user-defined function.

[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_MUG

LOGICAL

Flag to use the User Defined Function, USR_PROP_Mug, in model/usr_prop.f for calculating the gas phase viscosity, Mu_g.

.TRUE. ---------------------------- Call user-defined function.

[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_ROS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_ROs, in model/usr_prop.f for calculating the solids phase density, RO_s.

Applies to solids models: TFM

.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_CPS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_CPs, in model/usr_prop.f for calculating the solids phase constant pressure specific heat, C_ps.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_KS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Ks, in model/usr_prop.f for calculating the solids phase conductivity, K_s.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_DIFS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Difs, in model/usr_prop.f for calculating the solids phase diffusivity, Dif_s.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_MUS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Mus, in model/usr_prop.f for calculating the solids phase viscosity, Mu_s; second viscosity, lambda_s; and pressure, P_s.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_GAMA(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Gama, in model/usr_prop.f for calculating the gas-solids phase heat transfer coefficient, Gama_gs.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_FGS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Fgs, in model/usr_prop.f for calculating the gas-solids phase drag coefficient due to relative velocity differences, F_gs. Currently unavailable.

Applies to solids models: TFM
.TRUE. ------------------------------ Call user-defined function.
[*.FALSE.*] -------------------------- Use MFIX default calculation.

USR_FSS(Phase)

LOGICAL

Flag to use the User Defined Function, USR_PROP_Fss, in model/usr_prop.f for calculating the solids-solids phase drag coefficient due to relative velocity differences, F_ss. Currently unavailable.

Applies to solids models: TFM

.TRUE. ---------------------------- Call user-defined function.
[*.FALSE.*] ------------------------- Use MFIX default calculation.

C DOUBLE PRECISION
User defined constants.

C_NAME CHARACTER
Name of user-defined constant. (20 character max)

USR_DT(USR) DOUBLE PRECISION
Intervals at which subroutine write_usr1 is called.

USR_X_W(USR) DOUBLE PRECISION
Udf Hook: x coordinate of the west face or edge.

USR_X_E(USR) DOUBLE PRECISION
Udf Hook: x coordinate of the east face or edge.

USR_Y_S(USR) DOUBLE PRECISION
Udf Hook: y coordinate of the south face or edge.

USR_Y_N(USR) DOUBLE PRECISION
Udf Hook: y coordinate of the north face or edge.

USR_Z_B(USR) DOUBLE PRECISION
Udf Hook: z coordinate of the bottom face or edge.

USR_Z_T(USR) DOUBLE PRECISION
Udf Hook: z coordinate of the top face or edge.

USR_I_W(USR) INTEGER
Udf Hook: i index of the west-most cell.

USR_I_E(USR) INTEGER
Udf Hook: i index of the east-most cell.

USR_J_S(USR) INTEGER
Udf Hook: j index of the south-most cell.

USR_J_N(USR) INTEGER
Udf Hook: j index of the north-most cell.

USR_K_B(USR) INTEGER
Udf Hook: k index of the bottom-most cell.

USR_K_T(USR) INTEGER

Udf Hook: k index of the top-most cell.

USR_TYPE(USR) CHARACTER

Udf Hook: Type of user-defined output: Binary of ASCII.

USR_VAR(USR) CHARACTER

Udf Hook: Variables to be written in the user-defined output files.

USR_FORMAT(USR) CHARACTER

Udf Hook: Format for writing user-defined (ASCII) output file.

USR_EXT(USR) CHARACTER

Udf Hook: File extension for the user-defined output.

The `USR_` keywords do not have any explicit behavior. They are only basic input mechanisms to interact with user-defined functions.

For example, specifying `USR_X_w` does not result in the associated ‘I’ index, `USR_I_W` being calculated. It is upon the user to ensure that all user-hooks are fully specified.

8.13 Chemical Reactions

Chemical reactions are specified in the data file (`mfix.dat`) by providing species aliases and chemical equations. Rate expressions are specified in one of two user defined subroutines, `usr_rates.f` and `usr_rates_des.f`, respectively. Heats of reaction are automatically calculated. Optionally, users may specify constant heats of reaction in the data file.

An overview of using legacy **`rrates.f`** files is given at the end of this section. However**, this input method is no longer supported**.

8.13.1 Chemical Reactions Specification

There are five general steps to incorporating chemical reactions into a simulation:

1. Provide species names in the data file (SPECIES_G, SPECIES_S).

2. Assign a *unique identifier* (alias) to each species in the data file. (SPECIES_ALIAS_G and SPECIES_ALIAS_S)
3. Define chemical reaction parameters in the data file.
4. Define chemical reaction rates in `usr_rates.f` and/or `usr_rates_des.f`.
5. Use `make` to rebuild the MFIX executable.

Species names must appear **exactly** as given in the materials database (see the *Thermochemical Properties* section). Species names are typically 18 characters, and for some species, trailing spaces are needed.

The following explains steps 2-5 in more detail.

2. Each species must be assigned a *unique identifier* (alias).

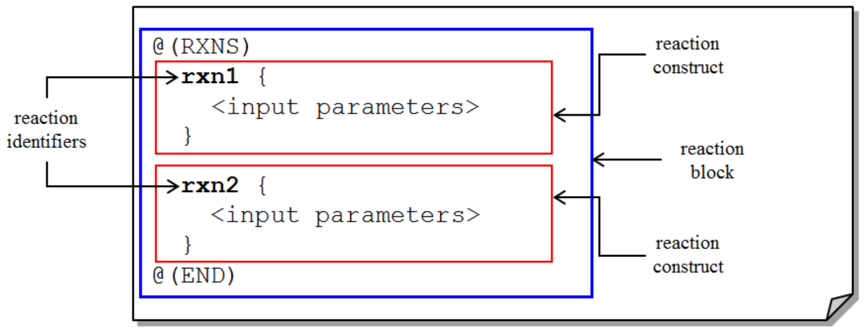
   Alias formatting restrictions:

   - Aliases must be unique.
   - Aliases are limited to 32 characters and must follow FORTRAN variable naming conventions (i.e., alphanumeric combinations with a letter as the first character).
   - Aliases are not case sensitive.
   - Aliases cannot conflict with existing MFIX variable names (e.g., a species alias of `MU_g` will cause an error when compiling MFIX).

3. Define chemical reactions in the data file using species aliases.

   Each reaction is identified by a *reaction construct*, and a *reaction block* is used to group reaction constructs in the data file. A reaction construct has the format, `rxn_name{…}`, where `rxn_name` is a *unique identifier* for the reaction. Reaction identifiers are limited to 32 characters and must follow FORTRAN variable naming convention.

   Reaction input format:



MFIX processes chemical reaction data differently than other input in the data file. A *reaction block* indicates the start and end of the reaction input. A *reaction construct* groups a single reaction's input parameters.

There are two reaction block types:

`@(RXNS)`…`@(END)` – indicates continuum phase chemical reactions (all TFM gas and solids phase reactions and DEM homogeneous gas phase reactions).

`@(DES_RXNS)`…`@(DES_END)` – indicates heterogeneous DEM chemical reactions (particle/gas).

A data file can only contain one reaction block of each type, whereas a reaction block must contain one or more reaction constructs.

The following keywords are available within a reaction construct.

CHEM_EQ CHARACTER

Chemical equation for the reaction constructed from species aliases. Example, Carbon combustion:

```
      CHEM_EQ = "C + 0.5O2 --> CO"
```

* A chemical equation of "NONE" deactivates the reaction during a simulation (e.g., `CHEM_EQ = "NONE"`)

DH DOUBLE PRECISION

User provided heat of reaction [cal/mole for CGS and J/kmole for SI].

fracDH DOUBLE PRECISION

The fraction amount of DH supplied to the indexed phase. By default, heats of reaction are automatically calculated and assigned to the appropriate phase(s). However, users may specify a constant heat of reaction, DH, for one or more reactions to override the automated calculations. If DH is given, then fracDH is required. The assigned fractional proportions must sum to one over all phases.

Reaction construct formatting notes:

- Chemical reactions are always specified as irreversible with reactants on the left and products on the right. (`CHEM_EQ = "Reactants --> Products"`)
- An arrow or equals sign can be used to distinguish reactants from products. (`Reactants --> Products` or `Reactants = Products`)
- Reversible reactions are specified as two irreversible reactions. *(see below example, Athermal, gas phase, reversible reaction)*
- Chemical equations may span several lines by including an ampersand (&) at the end of the line. As the example below illustrates, each line of the chemical equation is bound in quotation marks and the ampersand is located to the right of the second quotation mark.

```
@(RXNS)                                  ! Begin reaction block
  CH4_Combustion {                       ! Reaction 1 construct
    chem_eq = "CH4 + 2O2 --> " &         ! Chemical Reaction Line 1
      "CO2 + 2H2O"                       ! Chemical Reaction Line 2
  }                                      ! End reaction 1 construct
@(END)
```

- Chemical equations are limited to 512 characters.
- Chemical equations can be bound within single or double quotes. `CHEM_EQ = 'Reactants = Products'` or `"Reactants = Products"`)
- Catalytic reactions should contain a species from the catalyst phase in the chemical equation with a coefficient of zero. This insures the proper assignment of the heat of reaction. (`CHEM_EQ = 'A + 0.Cat -->3.0*R'` where `Cat` is a catalyst phase species)
- Catalyst phase species can be listed as a product, reactant, or both.

Several examples illustrating the data file input (steps 2 and 3) are provided below. Within the data input file comments are preceded with an exclamation mark (!).

Example: Methane Combustion: $\mathrm{CH_4}(g) + 2\mathrm{O_2} \rightarrow \mathrm{CO_2}(g) + 2\mathrm{H_2O}(g)$

Notes:

- Heat of reaction is automatically calculated (default).

```
NMAX_g = 4                               ! No. of gas phase species
Species_g(1) = "CH4 ANHARMONIC "         ! Methane
Species_g(2) = "O2"                      ! Oxygen
Species_g(3) = "CO2"                     ! Carbon dioxide
Species_g(4) = "H2O"                     ! Water Vapor

Species_Alias_g(1) = "CH4"               ! Methane
Species_Alias_g(2) = "O2"                ! Oxygen
Species_Alias_g(3) = "CO2"               ! Carbon dioxide
Species_Alias_g(4) = "H2O"               ! Water Vapor

@(RXNS)                                  ! Begin reaction block
  CH4_Combustion {                       ! Reaction 1 construct
    chem_eq = "CH4 + 2O2 --> CO2 + 2H2O" ! Chemical Reaction Eq
  }                                      ! End reaction 1 construct
@(END)                                   ! End reaction block
```

Example: Athermal, gas phase, reversible reaction: $\mathrm{A}(g) \leftrightarrow \mathrm{R}(g)$

Notes:

- Species database names and aliases are defined on single lines.
- The forward and backward reactions are defined separately.
- The heats of reaction are defined as zero (athermal) and explicitly assigned to the gas phase.

```
NMAX_g = 2                                ! No. of gas phase species
Species_g(1) = "A"  "R"                   ! Database names
Species_Alias_g(1) = "A" "R"              ! Species aliases

@(RXNS)                                   ! Begin reaction block
  fwd_AtoR {                              ! Reaction 1 construct
    chem_eq = "A --> R"                   ! Chemical Reaction Eq
    DH = 0.0                              ! (cal/moles-reacted)
    fracDH(0) = 1.0                       ! Gas phase HoR
  }                                       ! End reaction 1 construct
  rvs_AtoR {                              ! Reaction 2 construct
    chem_eq = "R --> A"                   ! Chemical Reaction Eq
    DH = 0.0                              ! (cal/moles-reacted)
    fracDH(0) = 1.0                       ! Gas phase HoR
  }                                       ! End reaction 2 construct
@(END)                                    ! End reaction block
```

Example - Char combustion: $\mathrm{C}(s) + 0.5\mathrm{O}_2(g) \rightarrow \mathrm{CO}(g)$

Notes:

- Species database names and aliases are defined on single lines.
- The heat of reaction is defined.
- The gas phase receives 20% of the heat of reaction.
- Solids phase 1 receives 80% of the heat of reaction.

```
NMAX_g = 2                                ! No. gas phase species

Species_g(1) = "O2" "CO"                  ! Database names
Species_Alias_g(1) = "O2" "CO"            ! Species aliases

NMAX_s(1) = 2                             ! No. solids phase species
Species_s(1,1) = "C(GR) REF ELEMENT"      ! Fixed Carbon (graphite)
Species_s(1,2) = "Coal Ash"               ! Coal Ash

Species_Alias_s(1,1) = "C" "Ash"          ! Fixed Carbon and Coal Ash

@(RXNS)                                   ! Begin reaction block
  Char_Combustion {                       ! Reaction 1 construct
    chem_eq = "C + 0.5O2 --> CO"          ! Chemical Reaction Eq
    DH = -52834.0                         ! (cal/moles-reacted)
    fracDH(0) = 0.2                       ! HoR assigned to gas phase
    fracDH(1) = 0.8                       ! HoR assigned to s. phase 1
  }                                       ! End reaction 1 construct
@(END)                                    ! End reaction block
```

Example – Compound DEM reaction:

CO combustion: $CO(g) + 0.5O_2(g) \rightarrow CO_2(g)$

CO2 gasification: $C(s) + CO_2(g) \rightarrow 2CO(g)$

Char combustion: $C(s) + 0.5O_2(g) \rightarrow CO(g)$

Notes:

- Gas phase species names and aliases are defined on the same line.
- Heats of reaction for all reactions are calculated automatically.
- A TFM reaction block is used for the gas phase homogeneous reaction.
- A DEM reaction block is used for gas/solids reactions.
- Reaction constructs are given in one line.

```
! Gas phase species data
  NMAX_g = 3
  Species_g(1) = "O2"    Species_Alias_g(1) = "O2"
  Species_g(2) = "CO"    Species_Alias_g(2) = "CO"
  Species_g(3) = "CO2"   Species_Alias_g(3) = "CO2"

! DES solids phase species data
  NMAX_s(1) = 2
  Species_s(1,1) = "C(GR) REF ELEMENT"
  Species_s(1,2) = "Coal Ash"

  Species_Alias_s(1,1) = "C"
  Species_Alias_s(1,2) = "Ash"

! Homogeneous gas phase reactions
  @(RXNS)
    CO_Combustion { chem_eq = "CO + 0.5O2 --> CO2" }
  @(END)

! DES Reaction block
  @(DES_RXNS)
    CO2_Gasification { chem_eq = "2.0C + O2 --> 2CO" }
    Char_Combustion  { chem_eq = "C + CO2 --> 2CO" }
  @(DES_END)
```

Additional comments:

- `Coal Ash` is not a species included in the thermochemical database and would require that the properties be given in the data file (see *Section 8.14 Thermochemical properties)*.
- One-line reaction constructs are only possible when the heat of reaction is automatically calculated (i.e., the chemical equation is the only input parameter).

4. Define chemical reaction rates in user defined function (UDF) files.
   - A reaction rate should be given in either `usr_rates.f` or `usr_rates_des.f` for each reaction listed in the data file.
   - All TFM gas and solids phase reactions as well as homogeneous gas phase reactions for DEM simulations are to be included in `usr_rates.f`. Reaction rates defined in `usr_rates.f` must have units of reacted moles per time per volume (i.e., moles/sec/cm^3 for CGS units and kmoles/sec/m^3 for SI units).
   - All discrete phase heterogeneous (particle/gas) reactions are to be included in `usr_rates_des.f` located in the des subfolder. Reaction rates defined in `usr_rates_des.f` must have units of reacted moles per time (i.e., moles/sec).

Formation and consumption rates are automatically calculated for each species from the reaction rate and chemical equation.

The rate in terms of reacted moles is related to the rates of formation and consumption through the stoichiometric coefficients. For example, consider homogeneous gas phase reaction of methane combustion:

$$\mathrm{CH_4} + 2\mathrm{O_2} \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O}.$$

The rate in terms of reacted moles, *Rate*, is related to the rates of formation and consumption as

$$Rate = \frac{-r_{CH_4}}{1}\left(\frac{mol_{\mathrm{CH_4}}/(s \cdot cm^3)}{mol_{\mathrm{CH_4}}}\right) = \frac{-r_{O_2}}{2}\left(\frac{mol_{\mathrm{O_2}}/(s \cdot cm^3)}{mol_{\mathrm{O_2}}}\right)$$
$$= \frac{r_{\mathrm{CO_2}}}{1}\left(\frac{mol_{\mathrm{CO_2}}/(s \cdot cm^3)}{mol_{\mathrm{CO_2}}}\right) = \frac{r_{\mathrm{H_2O}}}{2}\left(\frac{mol_{\mathrm{H_2}O}/(s \cdot cm^3)}{mol_{\mathrm{H_2O}}}\right),$$

where $-r_{CH_4}$ and $-r_{O_2}$ are the rates of consumption of methane and oxygen, and $r_{CO_2}$and r_{H_2O} are the rates of formation of carbon dioxide and water vapor, respectively.
Each reaction rate is assigned to the variable `RATES(rxn_name)`, where `rxn_name` is the reaction identifier used in the reaction construct. To minimize input errors when specifying reaction rates, species aliases (`SPECIES_ALIAS`) defined in the data file should be used in lieu of the associated species index.

For example, if oxygen is defined as gas phase species 2 with an alias of "`O2`", (e.g., `SPECIES_ALIAS_g(2)="O2"`)), when accessing gas phase species data for oxygen (e.g., molecular weight; MW_g), "`O2`" should be used and not the integer index 2, (e.g, `MW_g(O2)`).

Examples illustrating components of the UDF (step 4) are provided below.

Example: Methane Combustion: $\mathrm{CH_4}(g) + 2\mathrm{O_2} \rightarrow \mathrm{CO_2}(g) + 2\mathrm{H_2O}(g)$

Notes:

- Species database names and alias are defined on the same line.
- The fluid cell index (IJK) is passed as a dummy argument.
- Global field variables are referenced (RO_g, X_g, T_g, and EP_g)
- Species aliases (O2 and CH4) are used instead of the species indices.
- Reaction identifier (CH4_Combustion) is used in the rates array.
- Reaction rate is stored for post processing (see below).

mfix.dat:

```
NMAX_g = 4
Species_g(1) = "CH4 ANHARMONIC "  Species_Alias_g(1) = "CH4"
Species_g(2) = "O2"               Species_Alias_g(2) = "O2"
Species_g(3) = "CO2"              Species_Alias_g(3) = "CO2"
Species_g(4) = "H2O"              Species_Alias_g(4) = "H2O"

@(RXNS)
  CH4_Combustion { chem_eq = "CH4 + 2O2 --> CO2 + 2H2O" }
@(END)
```

usr_rates.f:

```
SUBROUTINE USR_RATES(IJK, RATES)

  DOUBLE PRECISION, INTENT(IN) :: IJK         ! Fluid Cell Index
  DOUBLE PRECISION, INTENT(OUT) :: RATES(:)   ! Reaction Rates
  DOUBLE PRECISION c_02  ! Oxygen concentration (mol/cm^3)
  DOUBLE PRECISION c_CH4 ! Methane concentration (mol/cm^3)

! Calculate species concentrations:
  c_O2  = (RO_g(IJK) * X_g(IJK,O2))/MW_g(O2)
  c_CH4 = (RO_g(IJK) * X_g(IJK,CH4))/MW_g(CH4)

! Methane Combustion
!---------------------------------------------------------------//
  RATES(CH4_Combustion) = 6.7d12 * exp(-2.4358d4/T_g(IJK)) * &
    EP_g(IJK) * (c_O2**1.3) * (c_CH4**0.2)

! Store the reaction rate for output/post processing.
  IF(CH4_Combustion <= NRR) &
    ReactionRates(IJK, CH4_Combustion) = RATES(CH4_Combustion)

END SUBROUTINE USR_RATES
```

Example: Athermal, gas phase, reversible reaction: $\mathrm{A}(g) \leftrightarrow \mathrm{R}(g)$

Notes:

- Species database names and alias are defined on the same line.
- The fluid cell index (IJK) is passed as a dummy argument.
- Global field variables are referenced (RO_g, X_g, T_g, and EP_g)

mfix.dat:

```
NMAX_g = 2                                 ! No. of gas phase species
Species_g(1) = "A" "R"                     ! Database names
Species_Alias_g(1) = "A" "R"               ! Species Aliases

@(RXNS)                                    ! Begin reaction block
  fwd_AtoR {                               ! Reaction 1 construct
    chem_eq = "A --> R"                    ! Chemical Reaction Eq
    DH = 0.0                               ! (cal/moles-reacted)
    fracDH(0) = 1.0                        ! Gas phase HoR
  }                                        ! End reaction 1 construct
  rvs_AtoR {                               ! Reaction 2 construct
    chem_eq = "R --> A"                    ! Chemical Reaction Eq
    DH = 0.0                               ! (cal/moles-reacted)
    fracDH(0) = 1.0                        ! Gas phase HoR
  }                                        ! End reaction 2 construct
@(END)                                     ! End reaction block
```

usr_rates.f:

```
SUBROUTINE USR_RATES(IJK, RATES)
  DOUBLE PRECISION, INTENT(IN) :: IJK       ! Fluid Cell Index
  DOUBLE PRECISION, INTENT(OUT) :: RATES(:) ! Reaction Rates
  DOUBLE PRECISION c_A ! species A concentration (mol/cm^3)
  DOUBLE PRECISION c_R ! species R concentration (mol/cm^3)

! Calculate species concentrations:
  c_A = (RO_g(IJK) * X_g(IJK,A))/MW_g(A)
  c_R = (RO_g(IJK) * X_g(IJK,R))/MW_g(R)

! Forward Reaction: A --> R (reacted moles/sec.cm^3)
!---------------------------------------------------------//
  RATES(fwd_AtoR) = 1.2d17 * exp(-5.837d3/T_g(IJK)) * &
    EP_g(IJK) * c_A

! Reverse Reaction: R --> A (reacted moles/sec.cm^3)
!---------------------------------------------------------//
  RATES(rvs_AtoR) = 2.5d41 * exp(-1.4897d4/T_g(IJK)) * &
    EP_g(IJK) * c_R

END SUBROUTINE USR_RATES
```

Example - Char combustion: $\mathrm{C}(s) + 0.5\mathrm{O}_2(g) \rightarrow \mathrm{CO}(g)$

Notes:

- The fluid cell index (`IJK`) is passed as a dummy argument.
- Algebraic expressions for the rate limiting steps are omitted for brevity.

mfix.dat: see step 3.

usr_rates.f:

```
SUBROUTINE USR_RATES(IJK, RATES)
  DOUBLE PRECISION, INTENT(IN) :: IJK        ! Fluid Cell Index
  DOUBLE PRECISION, INTENT(OUT) :: RATES(:)  ! Reaction Rates
      ⋮
! Rate limiting steps:
  DOUBLE PRECISION k_f   ! film diffusion       (cm/sec)
  DOUBLE PRECISION k_a   ! ash layer diffusions (cm/sec)
  DOUBLE PRECISION k_s   ! chemical kinetics    (cm/sec)
  DOUBLE PRECISION k_eff ! effective rate       (cm/sec)

! Total surface area of solids phase 1 in IJK
  DOUBLE PRECISION Sa  ! (cm^2/cm^3)

! C + 0.5O2 --> CO (reacted moles/sec.cm^3)
!---------------------------------------------------------//
! Verify that solids are present
  IF(.NOT.COMPARE(EP_g(IJK),ONE)) THEN
! Calculate film diffusion rate
    k_f = < film diffusion rate expression >   ! (cm/sec)
! Calculate ash diffusion rate
    k_a = < ash diffusion rate expression >    ! (cm/sec)
! Calculate kinetic rate rate
    k_s = < kinetic rate expression >          ! (cm/sec)

! Effective rate (cm/sec)
    k_eff = ONE/(ONE/k_a + ONE/k_f + ONE/k_s)

! Calculate total surface area of solids phase 1
    Sa = 6.0 * EP_s(IJK,1) / D_p0(1)
! Calculate the reaction rate.
    RATES(Char_Combustion) = 2.0 *(Sa * k_eff * Conc(O2))
  ELSE
! No solids --> No reaction
    RATES(Char_Combustion) = ZERO
  ENDIF
END SUBROUTINE USR_RATES
```

See `mfix-2016.1/model/tutorials/SpoutedBedCombustor` for details on a similar simulation setup.

Example – DES droplet evaporation: $H_2O(l) \rightarrow H_2O(g)$

Notes:

- Various algebraic expressions in the sample UDF are omitted for brevity.
- The global particle index (`NP`), phase index (`pM`), and fluid cell index (`IJK`) are passed as dummy arguments.

mfix.dat:

```
NMAX_g = 2                                ! No. of gas phase species
Species_g(1) = "Air" "H2O"                ! Database names
Species_Alias_g(1) = "Air" "Vapor"        ! Species Aliases

NMAX_s(1) = 1                             ! No. of solids phase species
Species_s(1,1) = "H2O(L)"                 ! Database names
Species_Alias_s(1,1) = "Liquid"           ! Species Aliases

@(DES_RXNS)
  Evap { Liquid --> Vapor }
@(DES_END)
```

usr_rates_des.f:

```
SUBROUTINE USR_RATES_DES(NP, pM, IJK, DES_RATES)
  DOUBLE PRECISION, INTENT(IN) :: NP    ! Global particle index
  DOUBLE PRECISION, INTENT(IN) :: pM    ! Particle solid phase
  DOUBLE PRECISION, INTENT(IN) :: IJK   ! Fluid Cell Index
  DOUBLE PRECISION, INTENT(OUT) :: DES_RATES(:)  ! Reaction Rates

!---------------------------------------------------------//
! Calculate the concentration gradient (mole/cm^3)
  Cmg_H2O = < expression for calculating gradient >

  IF(Cmg_H2O > ZERO) THEN
! Calculate mass transfer coefficient (cm/sec)
    H2O_xfr = < mass transfer coeff calculation >
! Calculate droplet surface area (cm^3)
    Sa = Pi * 4.0d0 * (DES_RADIUS(NP)**2)
! Calculate the mass transfer rate (moles/sec)
    DES_RATES(Evap) = Sa * H2O_xfr * Cmg_H2O
  ENDIF

! Store the reaction rate for post processing.
  IF(Evap <= NRR) ReactionRates(Evap) = &
    ReactionRates(IJK, Evap) + DES_RATES(Evap)

END SUBROUTINE USR_RATES_DES
```

See `mfix-2016.1/tests/dem-tests/evaporation` for additional details.

5. Use `make` to rebuild the MFIX executable.

   Detailed instructions on building the MFIX executable are given in earlier sections. Run `make` to rebuild `mfix` after making any of the following modifications:

   - Changing the number, order, or alias of any species in the data file.
   - Changing the number, order, or name of any chemical reaction in the data file.
   - Changing the chemical reaction rates in either `usr_rates.f` or `usr_rates_des.f`.

`make_mfix` preprocesses the data file to generated the `species.inc` file which is included within the `user_rates.f` and `usr_rates_des.f` files as code. Therefore changes in the data file may result in the executable being out of date.

This ends the extended explanation on the five general steps to incorporating chemical reactions into a simulation. Below is additional reaction information.

Write out reaction rates to SPx file:

1. In the data file, `mfix.dat`, set `NRR` to the desired number of reaction rates to be written out to the file `*.SPA`. This number is typically less than or equal to the total number of reactions.
2. In a reaction UDF (`usr_rates.f` or `usr_rates_des.f`) assign the desired reaction information to the variable `ReactionRates`. `ReactionRates` is a two-dimensional array. The first index references the fluid cell, `IJK`, while the second index ranges from `1` to `NRR`.

If the second index exceeds `NRR`, a run time error can result from over indexing the array. Using logical checks can eliminate potential errors!

Two of the above examples illustrate using the `ReactionRates` variable:

1. *Methane Combustion:* The calculated reaction rate is directly stored and a logical check is used to prevent over indexing of the `ReactionRates` array.
2. *DES droplet evaporation:* The calculated reaction rate is added to the storage array. Adding the calculated data to the storage variable is needed in DES since several discrete particles may exist in a single fluid cell. Again, a logical check is preformed to prevent over indexing the array.

Use an existing (legacy) `rrates.f` file:

The legacy `rrates.f` file should be copied to the run directory. Additionally, the following keywords should be specified in the data file:

USE_RRATES	LOGICAL
Flag to use legacy chemical reaction UDFs.	
SPECIES_NAME	CHARACTER
Names of gas and solids phase species as it appears in the materials database. The first NMAX(0) are the names of gas species. The next NMAX(1) are the names of solids phase-1 species, etc.	
NMAX	INTEGER
Number of species in phase m. Note that the gas phase is indicated as m=0.	

Legacy species keywords, `NMAX(m)` and `SPECIES_NAME(n)`, are **required** when using a legacy `rrates.f` file. Current species keywords `NMAX_g`, `NMAX_s`, `SPECIES_g`, and `SPECIES_s` **cannot** be used.

The only modification needed for a legacy `mfix.dat` and `rrates.f` file combination is the inclusion of `USE_RRATES=.TRUE.` in the data file.
An example of legacy file usage: `mfix-2016.1/tutorials/reactor1b`

Additional remarks:

- Building with chemical reaction support requires that the data file, `mfix.dat`, be present in the run directory as the species aliases and reaction identifiers are needed to construct a `species.inc` file.
- Species aliases and reaction identifiers must be unique. The build performs a cursory check on the supplied data and exits if non unique entries are identified.
- If any species alias or reaction identifier conflicts with an existing global variable in MFIX, an error will be reported and the code will fail to compile.

8.13.2 Stiff Chemistry Solver

A stiff chemistry solver has been fully integrated into MFIX. This approach first solves the convection/diffusion equations without chemical reaction source terms. A coupled set of ODEs is then directly integrated to impose chemical reactions effects. This approach may decrease simulation time by permitting larger time steps within the convection/diffusion model. However, the stiff chemistry solver may increase simulation time, especially if reactions are not stiff. Reactions are specified using the same approached outlined in the chemical reactions section.

The stiff chemistry solver is invoked by specifying the following keyword:

STIFF_CHEMISTRY LOGICAL

Flag to use stiff chemistry solver (Direct Integration).

STIFF_CHEM_MAX_STEPS INTEGER

Maximum number of internal steps ODEPACK may use to integrate over the time interval.Leaving this value unspecified permits an unlimited number of steps. Thee stiff solver reports the number of cells that exceed the number of steps as 'incomplete'.

The stiff chemistry solver does not support legacy rrates.f files

The stiff chemistry solver is not available with DES simulations.

Additional remarks:

- Variables governing ODE convergence criteria are specified as parameters in `stiff_chem_mod.f` found in the `model/chem` directory. Additional information on these parameters and there usage is available in `model/ODEPACK.F`.
- It is recommend to first run your simulation in debug mode. This will catch some common programmatic errors in the `usr_rates.f` file. Additionally, the stiff chemistry solver checks for NaNs calculated in the `usr_rates.f` file.
- The tutorial located in mfix-2016.1/tutorials/silane_pyrolysis shows how to use the stiff chemistry solver.

8.14 Thermochemical Properties

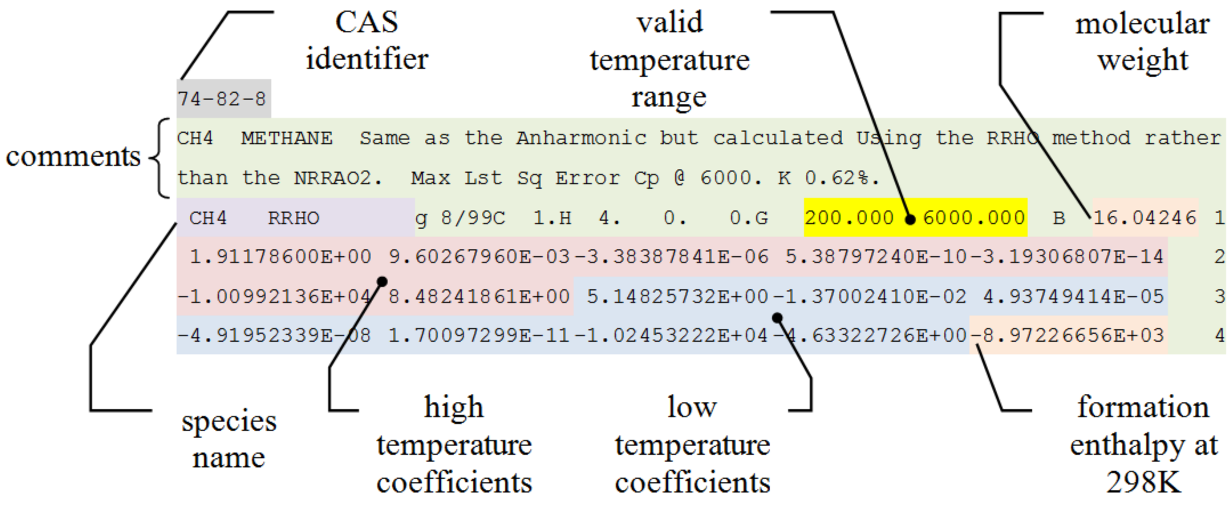
The directory `mfix-2016.1/model/thermochemical` contains the database of Burcat and Ruscic (2005) and routines for reading the database. With linkage to this database the users need not manually enter data for molecular weight, specific heat, and heats of reactions. Instead the users only need to enter the names of the species (keyword `SPECIES_g` and `SPECIES_s`) in the data file. If such information is already provided in either the data file or a `BURCAT.THR` file in the run directory then MFIX will not reference the database. That is, MFIX reads the necessary thermo-chemical data from files in the following order:

1. `mfix.dat`
2. `BURCAT.THR` file in the run directory

3. `mfix-2016.1/model/thermochemical/BURCAT.THR`.

The species names are case sensitive and should match the names in BURCAT.THR exactly; alternatively aliases can be defined for common species, such as `O2`, in `read_therm.f`. See `mfix-2016.1/tests/thermo` for a sample case that accesses the database. The format of `BURCAT.THR` file resembles CHEMKIN format, but with several notable differences. To include thermochemical data in the mfix.dat file then this information must start below a line that starts with `THERMO DATA`.

Example dataset from `BURCAT.THR` with notations:



```
74-82-8
CH4   METHANE  Same as the Anharmonic but calculated Using the RRHO method rather
than the NRRAO2.  Max Lst Sq Error Cp @ 6000. K 0.62%.
 CH4   RRHO          g 8/99C  1.H  4.   0.   0.G  200.000  6000.000  B  16.04246 1
 1.91178600E+00 9.60267960E-03-3.38387841E-06 5.38797240E-10-3.19306807E-14    2
-1.00992136E+04 8.48241861E+00 5.14825732E+00-1.37002410E-02 4.93749414E-05    3
-4.91952339E-08 1.70097299E-11-1.02453222E+04-4.63322726E+00-8.97226656E+03    4
```

CAS identifier
valid temperature range
molecular weight
comments
species name
high temperature coefficients
low temperature coefficients
formation enthalpy at 298K

Each entry in the database starts with a unique CAS identifier (`74-82-8`) for the species, followed by several lines of comments highlighted in green. The data section starts with the species name in columns 1-18 (`CH4      RRHO`). Common species names may be followed by strings (RRHO) that identify the method used to determine the coefficients. Additional information follows the species name. The numbers toward the end of the line are the temperature limits (`200.000   6000.000`) in degrees Kelvin where the property calculation is valid and the molecular weight (`16.04246`). Unlike CHEMKIN the common temperature for the high and low temperature branches are not recorded; it is always 1000 K. The next three lines give the fourteen coefficients (seven coefficients each for the high and low temperature branches) and the formation enthalpy at 298 K (which is also not included in CHEMKIN format). All the coefficients and the enthalpy of formation are normalized with the gas constant R (cal/mol/K). The low temperature coefficients (a_L) should be used for temperatures in the range T_{low} to 1000K and the high temperature coefficients (a_H) should be used for temperatures in the range 1000K to T_{high}. The coefficients are stored in a fixed format (E15.0) as follows:

a_H^1	a_H^2	a_H^3	a_H^4	a_H^5
a_H^6	a_H^7	a_L^1	a_L^2	a_L^3
a_L^4	a_L^5	a_L^6	a_L^7	ΔH_f°

where ΔH_f° is the formation enthalpy at 298K.

The normalized specific heat is given by

$$C_p/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4.$$

Additional database comments:

- A number of species in the database have a lower temperature limit of 300K which is 2 degrees above the reference temperature (298 K) used for formation enthalpy calculation. For those species MFIX relaxes the lower limit for Cp calculations to 298 K to enable heat of reaction calculation. see `read_database.f`
- The database reader is set up such that the database is read only if necessary.
- For additional details see the Burcat and Ruscic (2005) report located in the thermo-chemical subdirectory, `mfix-2016.1/model/thermochemical/intro.pdf`.

If you include thermochemical properties in mfix.dat all keywords defined below the line that starts with THERMO DATA will be ignored!

8.15 Parallelization Control

The parallel performance depends on several things and one has to evaluate different options before choosing the right strategy for the problem at hand. For example if the J direction is the strongest coupled direction, the preconditioning for the linear solver will be poor if there is decomposition in that direction. However, since decomposing in all the directions reduces the processor grid surface area, the communication cost will be less for the same computational grid. The preconditioners are chosen with the keyword LEQ_PC. In addition to LINE relaxation, one can choose the "DIAG" or "NONE" preconditioner that reduces inter-processor communications but would increase the number of linear equation solver iterations. The DIAG and NONE choices for preconditioners may be appropriate for all equations except the continuity (or pressure and volume fraction correction) equations. The parallel performance is greatly dependent on the choices stated here, and some trial an error may be required to determine the right combination of decomposition direction and the choice of preconditioners to get the best performance in production runs.

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.

NODESI Number of grid blocks in x-direction. .	INTEGER
NODESJ Number of grid blocks in y-direction.	INTEGER
NODESK Number of grid blocks in z-direction.	INTEGER
SOLVER_STATISTICS Print out additional statistics for parallel runs	LOGICAL
DEBUG_RESID Group residuals to reduce global collectives.	LOGICAL
ENABLE_DMP_LOG All ranks write error messages.	LOGICAL
DBGPRN_LAYOUT Print the index layout for debugging.	LOGICAL

By default, the MFIX attempts to distribute computational cells evenly across all MPI ranks. However, this may not be ideal in all cases (i.e., Cartesian cut-cell simulations and/or MFIX-DEM simulations).

Manually specifying partition sizes

Consider the following mesh and domain decomposition:

mfix.dat (*excerpt*)

```
# Geometry
IMAX =  30
JMAX = 100
KMAX =  30

# Domain Decomposition
NODESI = 2
NODESJ = 4
NODESK = 2
```

To concentrate processors at the bottom of the domain, one could specify the following in a file named gridmap.dat in the run directory.

```
  2    4     2     ! NODESI, NODESJ, NODESK
  0     15
  1     15
  0     10
  1     10
  2     10
  3     70
  0     15
  1     15
```

- The first line is the decomposition (2x4x2).
- The next 2 lines are the decomposition sizes in the x-direction (15, 15).
- The next 4 lines are the decomposition sizes in the y-direction (10, 10, 10, 70).
- The last 2 lines are the decomposition sizes in the z-direction (15, 15).

This is a manual and static decomposition and you will need to adjust it to get the best results.

Calculated partition sizes

For simulations containing a significant amount of cut-cells, the following flags enable the code to calculate an optimal domain decomposition:

mfix.dat (excerpt)

```
RE_INDEXING = .TRUE.
REPORT_BEST_DOMAIN_SIZE = .TRUE.
```

MFIX will go through the pre-processing, report the best decomposition and save the result in the file suggested_gridmap.dat. You can review this file and if it makes sense, rename it as gridmap.dat and start the simulation again with this decomposition (set

REPORT_BEST_DOMAIN_SIZE = .FALSE. to avoid MFIX quitting after the pre-processing). This optimized gridmap is based on the Eulerian mesh and is not yet adapted for DEM (i.e. it doesn't take into account the particle location).

8.16 Batch Queue Environment

MFIX can be used on systems where code execution is controlled through batch queue submission system instead of interactive or background job type methods shown in the previous section. Usually the user specifies the wall clock time duration of the job and batch queuing system prioritize incoming jobs based on their resource allocation requests. In order for MFIX to avoid abrupt and abnormal termination at the end of the batch job session, several keywords need to be entered in mfix.dat. Controlled and clean termination in environments with batch queue is important as the system may terminate the batch job while MFIX is writing out *.SP files, which may corrupt the files or cause loss of data.

For this purpose, MFIX checks whether the user-specified termination criteria is reached at the beginning of each time step. However, to avoid performance bottlenecks on small systems where the user is running their jobs without a batch queue, this feature is disabled by default. In order to enable this feature the following block of commands need to be entered in mfix.dat.

```
CHK_BATCHQ_END = .TRUE.    ! Enable the controlled termination feature
BATCH_WALLCLOCK = 3600.0   ! Specify the total wall clock duration
                           ! of your job in seconds
TERM_BUFFER = 300.0        ! Specify a buffer time to start
                           ! clean termination of MFIX
```

Setting `CHK_BATCH_END = .TRUE.` in mfix.dat will enable the checking of the termination criteria at the beginning of each time step. In the above example, the user has set the total wall clock time for the duration of the batch session to 1 hour (this is specified in seconds in mfix.dat) and a buffer of 300 seconds has been set so that MFIX has sufficient time to terminate cleanly by writing out all *.SP and *.RES files before the batch session terminates. The duration of the buffer is critical for simulations with large files. MFIX will check if `elapsed time >= (BATCH_WALLCLOCK – TERM_BUFFER)` to start clean termination.

Another way to gracefully terminate MFIX as soon as possible is to create an empty file named `MFIX.STOP` (filename all uppercase) in the working directory where MFIX runs. At the beginning of each time step if `MFIX.STOP` file is detected to exist, then MFIX will terminate gracefully by saving `*.RES` files. `CHK_BATCHQ_END` flag must be set to `.TRUE.` in order to activate this feature.

The following command can be used to gracefully terminate MFIX:

```
> touch MFIX.STOP
```

Remember to erase the file once MFIX terminates, otherwise the next time MFIX is run in the same directory it will terminate immediately.

```
> rm -f -r ./MFIX.STOP
```

CHK_BATCHQ_END

LOGICAL

Enables controlled termination feature when running under batch queue system to force MFIX to cleanly terminate before the end of wall clock allocated in the batch session.

BATCH_WALLCLOCK

DOUBLE PRECISION

Total wall-clock duration of the job, in seconds.

TERM_BUFFER

DOUBLE PRECISION

Buffer time specified to allow MFIX to write out the files and cleanly terminate before queue wall clock time limit is reached such that (BATCH_WALLCLOCK-TERM_BUFFER) is less than then batch queue wall clock time limit, in seconds.

9 MFIX in Other OS Environments

MFIX is developed for and tested on Linux systems. Support for building and running MFIX on other operating systems is extremely limited. This section provides options for users that do not have access to a Linux system. Using Cygwin or a virtual Linux machine still requires basic knowledge of Linux operation.

9.1 Prebuilt Windows binaries for MFIX

A prebuilt serial MFIX binary for running on Windows systems is available on the download page (https://mfix.netl.doe.gov/mfix/download-mfix). The prebuilt binary is sufficient unless the MFIX simulation includes user defined files (usr*.f) or chemical reactions.

Additional information is available on the website and in the mailing list archives.

9.2 Building MFIX on Windows with Cygwin

Cygwin can be used to build a native Windows executable. An overview of the steps to build MFIX under Cygwin is given below.

9.2.1 Installing Cygwin

2. Download the Cygwin installer setup-x86.exe (32-bit installation) or setup-x86_64.exe (64-bit installation) from http://www.cygwin.com/.
3. Run the installer (if you do not have Windows administrator rights, run the installer on the command line with the "--no-admin" option.)
4. Select the default install options
5. At the installation step "Select Packages", install the packages:
    - gcc-fortran
    - autoconf
    - automake
    - make
    - diffutils
    - sed
6. You can rerun the Cygwin installer anytime if you want to install additional development tools.

9.2.2 Building and Running MFIX

Once Cygwin is installed, the build process is the same as on Linux. See the section "Building MFIX" for more details.

1. Download MFIX source tarball

2. Extract the tar ball

```
> tar xzf mfix-2016.1.tar.gz
```

3. Go to fluidbed1 tutorial

```
> cd mfix-2016.1/tutorials/fluidbed1
```

4. Configure and build MFIX

```
> ../../configure_mfix && make
```

5. Run MFIX for the fluidbed1 tutorial. Note that on Windows, the mfix.exe executable has an extension ".exe".

```
> ./mfix.exe
```

   (Optional) To run MFIX in the background

```
> nohup ./mfix.exe > run.log&
```

   While it is running in the background, you can follow the output with:

```
> tail -f out1
```

If you have problems building or running MFIX in Cygwin, check the mailing list archives to see if your question has already been answered. Information on the mailing lists and mailing list archives are provided at the end of this document.

9.3 Building MFIX on Mac OS X with Homebrew

Homebrew is the easiest way to install MFIX build dependencies. (Other OS X package managers are Fink and MacPorts.)

9.3.1 Installing Homebrew

7. Go to http://brew.sh and follow the installation instructions.
8. Once homebrew is installed, install MFIX build dependencies with the command:

```
> brew install gcc autoconf automake make gnu-sed
```

9.3.2 Building and Running MFIX

Once Homebrew is installed, the build process is the same as on Linux. See the section "Building MFIX" for more details.

Note: when building with ifort on OS X, you may get an error unless you override RANLIB because the OS X ranlib does not include the -c option by default.

```
> ../../configure_mfix FC=ifort RANLIB='ranlib -c' && make
```

If you have problems building or running MFIX on OS X, check the mailing list archives to see if your question has already been answered. Information on the mailing lists and mailing list archives are provided at the end of this document.

9.4 Use a virtual Linux machine

Virtual machines are another method of running MFIX may be run on Windows and Mac OS X. This approach requires that a virtualizer be installed on your system such as VirtualBox or VMWare with a Linux guest operating system. The procedure outlined in section 4 can be used on the virtual Linux machine to install MFIX.

10 Mailing lists

Several mailing lists are available to communicate among MFIX users and developers. When your subscription to MFIX is accepted, you are automatically added to the mfix-news mailing list, where important announcements about MFIX are shared with the MFIX community.

The most widely used mailing list is mfix-help, which allows users to post questions and eventually help other users with similar issues.

The mailing list home page is located at https://mfix.netl.doe.gov/sympa. Click on the "List of lists" tab to view all available mailing lists. Most of them have a very low bandwidth, and most users only subscribe to the mfix-help list.

Once you subscribe to a list, you can send/receive messages to/from the MFIX community. You can also search archived messages to see if there is already a solution to a common problem.

There are many options to manage your subscription, including subscribing, unsubscribing, and choosing the delivery mode.

Please visit https://mfix.netl.doe.gov/sympa/help/user to view the mailing list user guide.

Mailing list etiquette:

1) Please allow sufficient time (say 2 to 3 business days) for MFIX developers and users to reply before posting unanswered questions again.

2) Unless prior arrangement has been made with a given MFIX developer, do not send requests directly to the developer, but send the request to the appropriate mailing list instead. This ensures proper archiving of the thread and provides better opportunity for everyone to reply. Follow-up questions should also be sent to the mailing list.

3) Do not ask for a copy of a reference, e.g., a journal article.

4) Prior to submitting help requests regarding MFIX installation or compilation issues, please check the archives of mfix-help and if you are still having a problem, email mfix-help@mfix.netl.doe.gov by providing the following important details in your message after the description of the problem encountered:
   a. MFIX version you are trying to install or run
   b. Some details on your operating system environment (for Linux: copy and paste the response of uname –a command, Linux distribution name and version also)
   c. Your compiler name and version number (e.g. ifort -v will give the version number for Intel fortran compiler)

d. Output for your $PATH environment (in csh type echo $PATH)
e. Your MPI library name and version number (if compilations problem with DMP mode encountered but make sure you can compile and run a simple hello world type MPI program with your current installation) Also please provide hardware details such as number of cores per socket in your system (or send the output for "cat /proc/cpuinfo" and how many cores you are trying to utilize.

Common reasons you may not receive an answer to your request

1. You did not subscribe to the mailing list.
2. You sent the request to an individual and not to the mailing list.
3. Your question has already been answered and is available in the archive.
4. You did not provide sufficient description of your problem (saying "It doesn’t work" is not useful).
5. Your question is outside the scope of the mailing list.

11 User contribution

If you wish to contribute to the development of MFIX, please contact the MFIX team at admin@mfix.netl.doe.gov. We are looking for simulation results (figures, animations, input files, user-defined subroutines), and new models that could benefit the entire MFIX community. If you have written or know any publication that uses MFIX, please let us know and we will post the citation on the website (https://mfix.netl.doe.gov/publications/publications-citations/). Proper credit will be given to all contributors.

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