CCSI Pulverization Model

User Manual

Version 2.0.0

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To obtain support for the products within this package, please send an e-mail to ccsi-support@acceleratecarboncapture.org.

CCSI CFD Models

1.0 ABSTRACT

CCSI Attrition and Pulverization Model: Particle attrition is frequently encountered during the processing and handling of mesoporous particles in chemical processing, where the particles suffer progressive loss of material as a result of collisions and friction. In fluidized bed reactors, particle size reduction due to attrition can result in agglomeration and poor fluidization, and the generation of fine debris may further constitute health hazards, leading to environmental pollution. A discrete element method (DEM)-based attrition model was developed to investigate the attrition of initially monodispersed solid particles in a jet cup. Particle size reduction due to chipping and abrasive wear from particle-particle and particle-wall interactions were considered and explicitly implemented into the simulation. The attrition models can be used to study the effects of operational factors, such as jet velocity, particle size, solid density, and jet cup design on the attrition propensity. The Coal Pulverization Model, which was developed by extending the CCSI DEM-based modeling capability, is included here.

2.0 REPORTING ISSUES

To report an issue, please send an e-mail to ccsi-support@acceleratecarboncapture.org.

3.0 VERSION LOG

Product	Version Number	Release Date	Description
MFIX-DEM Pulverization Model	2.0.0	03/31/2018	Initial Open Source Release
MFIX-DEM Pulverization Model	2014.10.0	10/31/2014	2014 October IAB Release

MFIX-DEM Pulverization Model

1.0 INSTALLATION

The installation of the Coal Pulverization Discrete Element Model (DEM) generally follows the Multiphase Flow with Interphase eXchanges (MFIX) manual [1]. The present document solely intends to provide an overview on specific procedures required to enable the Pulverization-DEM module within MFIX. Please refer to the MFIX User Manual [1] for additional details.
Note: The current Pulverization-DEM module only works with the MFIX-2012-1 version.

1.1 Prerequisites

The same hardware and software environments that are specified by MFIX [1] apply.

1.2 Third Party Software

The open-source, multi-platform data analysis and visualization application *ParaView* is recommend for post-processing of the MFIX simulation and can be downloaded online at: http://www.paraview.org. Other similar visualization software (for example, *Tecplot*®, *VisIt*) can also serve the same purpose.

1.3 Product Installation

It is assumed that the user has downloaded the MFIX source files and created the entire MFIX directory (for example, `$HOME/mfix`) in the Linux® system. Currently, the Intel® Fortran compiler is recommended to be used for the installation.

The source codes and the simulation input files for the Pulverization-DEM model are distributed as a tar ball `Pulverization.tar.gz`. Download the tar ball into the MFIX directory, and then extract the tar ball into a run folder `$HOME/mfix/pulverization` by typing:

```
tar xvf Pulverization.tar.gz
```

Three subdirectories are created: `model` contains the Pulverization-DEM module files, `test` contains the example input files, and `results` contain the standard output files.

Copy all of the contents within the `$HOME/mfix/pulverization/model` folder into the `$HOME/mfix/pulverization` folder by typing:

```
cp -r $HOME/mfix/pulverization/model/* $HOME/mfix/pulverization/
```

Move the following files from the `$HOME/mfix/pulverization` folder to the `$HOME/mfix/model` folder to replace the original files:

```
mfix_l.make

mfix_l_not.make

mfix_u.make

mfix_u_not.make
```

Copy the desnamelist.inc and calc_attrition_des.f files from the $HOME/mfix/pulverization/des folder to the $HOME/mfix/model/des folder by typing:

```
mv –f mfix_l.make mfix_l_not.make mfix_u.make mfix_u_not.make
   $HOME/mfix/model


cd $HOME/mfix/pulverization/des


cp –f desnamelist.inc calc_attrition_des.f $HOME/mfix/model/des


cd ..
```

Follow the MFIX instructions [1] to build the mfix executable in the `$HOME/mfix/pulverization` folder.

```
sh $HOME/mfix/model/make_mfix
```

Select “Yes” for “Force re-compilation of source files in run directory”. Upon a successful build, a custom mfix.exe is available in the $Home/mfix/pulverization folder.

2.0 SIMULATIONS

The Pulverization-DEM model input files `mfix.dat` and `particle_input.dat` are included in the `$Home/mfix/pulverization/test` folder, where a 2D spherical coal with a diameter ~0.2 cm is represented by assemblies of discrete elements with a uniform diameter of ~75 μm, and is subjected to vertical compression from a rigid plate resembled by a horizontal array of pseudo particles.
Note: The present model is currently limited to serial computation.

Simulation results can be viewed in ParaView by loading the .pvd file and then applying the “Glyph” filter where the “Glyph Type” should be changed to “Sphere”, “Orient” selected, “Scale Mode” should be changed to “scalar”, and the “Set Scale Factor” is suggested to be “1”. The damage evolution within the coal can be visualized by changing the legend from “Diameter” to “Fcohesive”, which indicates whether a particle is bonded (Fcohesive=1) or not bonded (Fcohesive=0).

The transient load response is recorded in the output file “`Monitor_Stress.dat`”, in which the first column corresponds to the time, the second column corresponds to the tangential force, and the third column is the normal force. A time-load plot can be obtained as pictured in Figure 5:

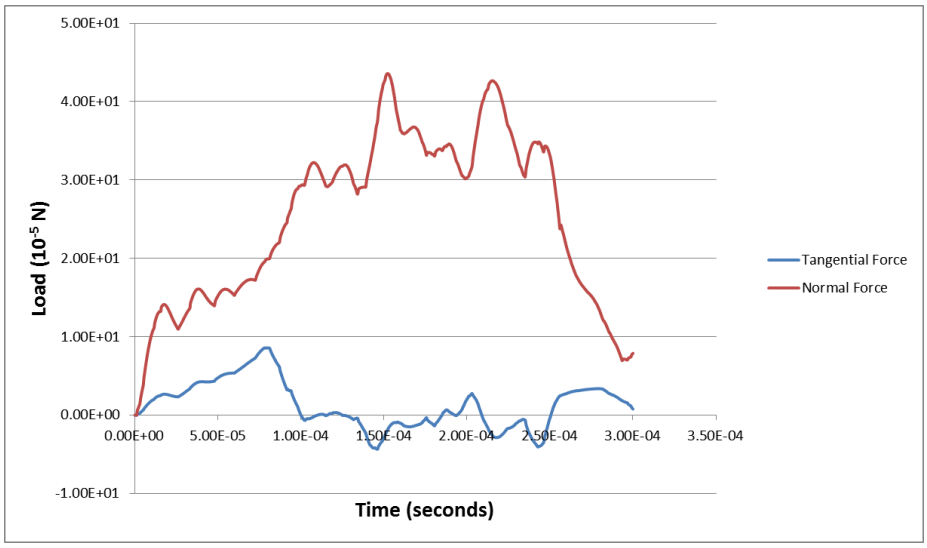

Figure 1: Transient load response (Intel Fortran compiler used).

The standard output results are contained in the `$Home/mfix/pulverization/results` folder.

3.0 REFERENCES

4.0 [1] MFIX – MULTIPHASE FLOW WITH INTERPHASE EXCHANGES, VERSION MFIX-2012-1, JANUARY 2012. (THE README.PDF IS DISTRIBUTED WITHIN THE MFIX TAR BALL.)