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# **Software Requirements Specification**

**for**

# **MFIX-User Interface**

**Version 1.0**

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## Revision History

Name	Date	Reason For Changes	Version

# 1. Introduction

## Purpose

This SRS outlines the requirements for MFIX-UI version 1.0.

## Document Conventions

Place holder.

## Intended Audience and Reading Suggestions

The intended audience for this document is primarily project managers, GUI developers, and MFIX users. The secondary audience will be code testers, and documentation writers. This primary purpose of the document is to capture the design and performance specifications in one location so that the project scope can be defined and managed.

## Product Scope

A comprehensive graphical user interface (GUI) for interacting with the MFIX Suite of multiphase flow software will be developed. The purpose of the GUI will be to provide a user-friendly interface to:

- Set up the MFIX simulation;
- Control and interact with the MFIX code during execution;
- Provide post-processing capabilities for analyzing output data;

While developing this capability in V1.0, we will monitor progress of other development teams that are also creating MFIX enhancements (MFIX Development, REMS toolkit development, UQ toolkit development) and provide these groups with information on GUI capabilities and incremental GUI code beta releases.

## References

Place holder text.

# 2. Overall Description

## Product Perspective

This product is an evolution of the current MFIX-GUI application. The original product (v0.1) is currently available to the MFIX user base and works as a mediator between users and the model deck file (mfix.dat) while offering moderate runtime analysis (e.g., plotting residuals) and build environment support. The expanding model capabilities of the MFIX software suite, growing need for runtime control and interaction of simulations, and model optimization necessitates an immersive user interface.

## Product Functions

- Fully specify an MFIX simulation through an easy to use user interface (UI)
  - Define run parameters, geometry, initial/boundary conditions, material properties
  - Basic in situ 'sanity checks' on specified input
- Instantaneous control/interaction of a running MFIX simulation
  - Launch simulations from the UI, locally or via a queuing system
  - Connect to running simulations that were launched in batch mode
  - Patch field variables with user specified value
- Basic in situ data collection/analysis
  - Average field variable across point/line/plane/volume
  - Plot field variable across line/plane

## User Classes and Characteristics

**General CFD practitioners:** This user class is comprised of traditional CFD users interested primarily in setting up and running single- and multi-phase flow simulations. This class may make use well supported/defined UDF hooks however; substantial interest in code development is not expected.

**General developers:** This user class is comprised of researches at Universities and other National Labs. This class engages in moderate levels of code development, primarily to investigate specific physical models. This class needs the ability to readily build and rebuild MFIX executables from locally modified source code. This user is not like to modify the MFIX-UI or contribute to general code maintenance.

**MFIX developers:** This user class is comprised of the core MFIX development team and NETL support collaborators. This class will regularly modify the MFIX solver source code for debugging and model development. This class requires access to the MFIX deck file for toggling new features. This user must work tightly with the MFIX-UI team to ensure features added to the solver are available through the MFIX-UI.

## Operating Environment

The user interface shall work on the following operating systems:

- Linux (Ubuntu, Fedora, OpenSUSE)
- Windows 7, 8.1, 10
- OS X (Mac)

The interface shall connect and interact with running models on Linux based systems. Joule, the NETL Supercomputer, is the primary target of this feature. However, extension and testing on other HPC systems will be investigated as access and resources permit.

## Design and Implementation Constraints

Python will be used to implement the MFIX-UI. The MFIX executable compiled with Python/Fortran bindings provides access to Python libraries for networking. Anaconda Python Distribution from Continuum Analytics provides dependencies across all operating environments as described in 0.

- Primary Language: Python
  - Target versions: 2.7 and 3.5

- This includes all “python core” libraries such as os, etc.
- Third party Python libraries (open source)
  - GUI library: Qt
    - Supported wrappers: PyQt4, PyQt5, PySide
  - 3D graphics library: VTK
  - Array library: numpy
  - Fortran/Python interface generator: F2PY
  - Web framework library: Flask

## User Documentation

Text based documentation generated using Sphinx, covering the following areas:

- Disclaimer
- Introduction
- Installation
- Features
- Tutorials
- Developer Guide
  - Contributing
  - Style Guide
  - Tests
  - Building Binaries
- Help
- Release Notes
- Test Harness Report
- API
  - Automatically pulled from docstrings in the code

Video based screen cast tutorials will also be developed and published on YouTube through the NETL YouTube Channel.

## Assumptions and Dependencies

This plans assumes continued support for the Anaconda Python Distribution and that it will contain the following dependencies:

- PyQt4, PyQt5, or PySide
- VTK
- *Numpy*
- F2PY
- Flask

## 3. External Interface Requirements

### User Interfaces

The UI consists of a basic layout with a *main menu bar*, tabbed *graphics windows*, a *mode area*, *mode selection bar*, and a *console*, illustrated in Figure 1. Splitters will resize/hide the mode area

and the graphics area as well as hide/resize the console. Widgets listed in the *mode area* will change based on the user model selections.

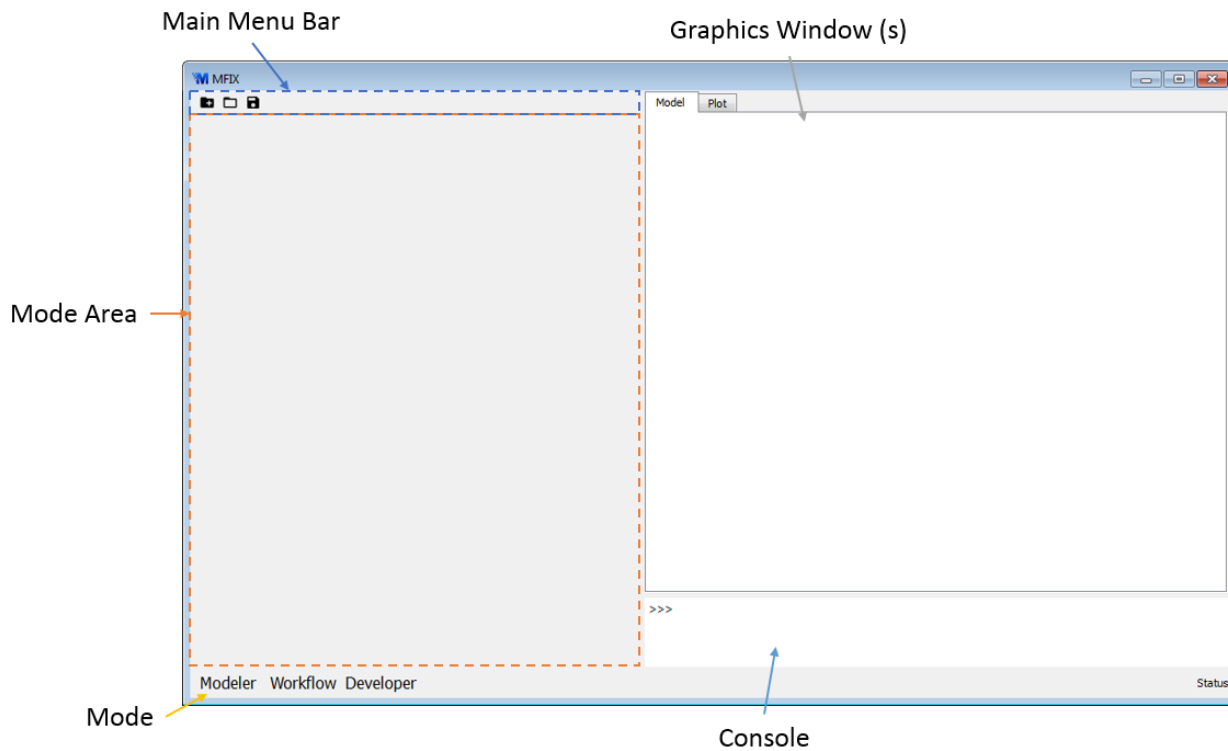
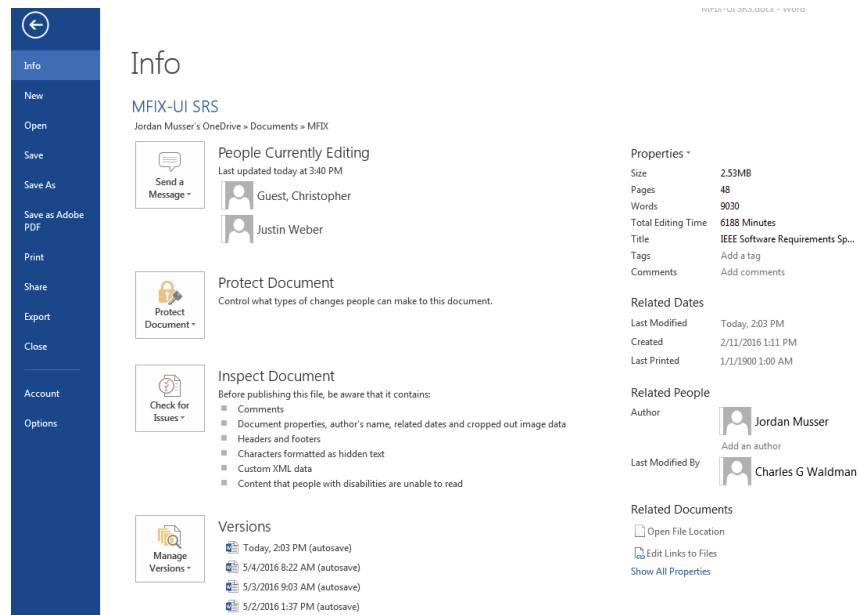


Figure 1: Basic layout of UI

### 3.1.1 File Menu

The file menu should provide pertinent information regarding the project, similar to MS office. The following information should be displayed:

1. Author
2. Last date modified
3. Directory size on disk?



*MS Word's version of the file menu*

### 3.1.2 Modeler Mode

Modeler mode intuitively guides a user through creating an MFIX model. Shown in Figure 2, the interface consists of a “Navigation Pane” and a “Task Pane”**Error! Reference source not found.**the user through the model setup process in a logical order. The entries in this tree adapt to user input, i.e. hiding/showing entries based on user selected options and models. the user through the model setup process in a logical order. The entries in this tree adapt to user input, i.e. hiding/showing entries based on user selected options and models. the user through the model setup process in a logical order. The entries in this tree adapt to user input, i.e. hiding/showing entries based on user selected options and models. the user through the model setup process in a logical order. The entries in this tree adapt to user input, i.e. hiding/showing entries based on user selected options and models. the user through the model setup process in a logical order. The entries in this tree adapt to user input, i.e. hiding/showing entries based on user selected options and models.

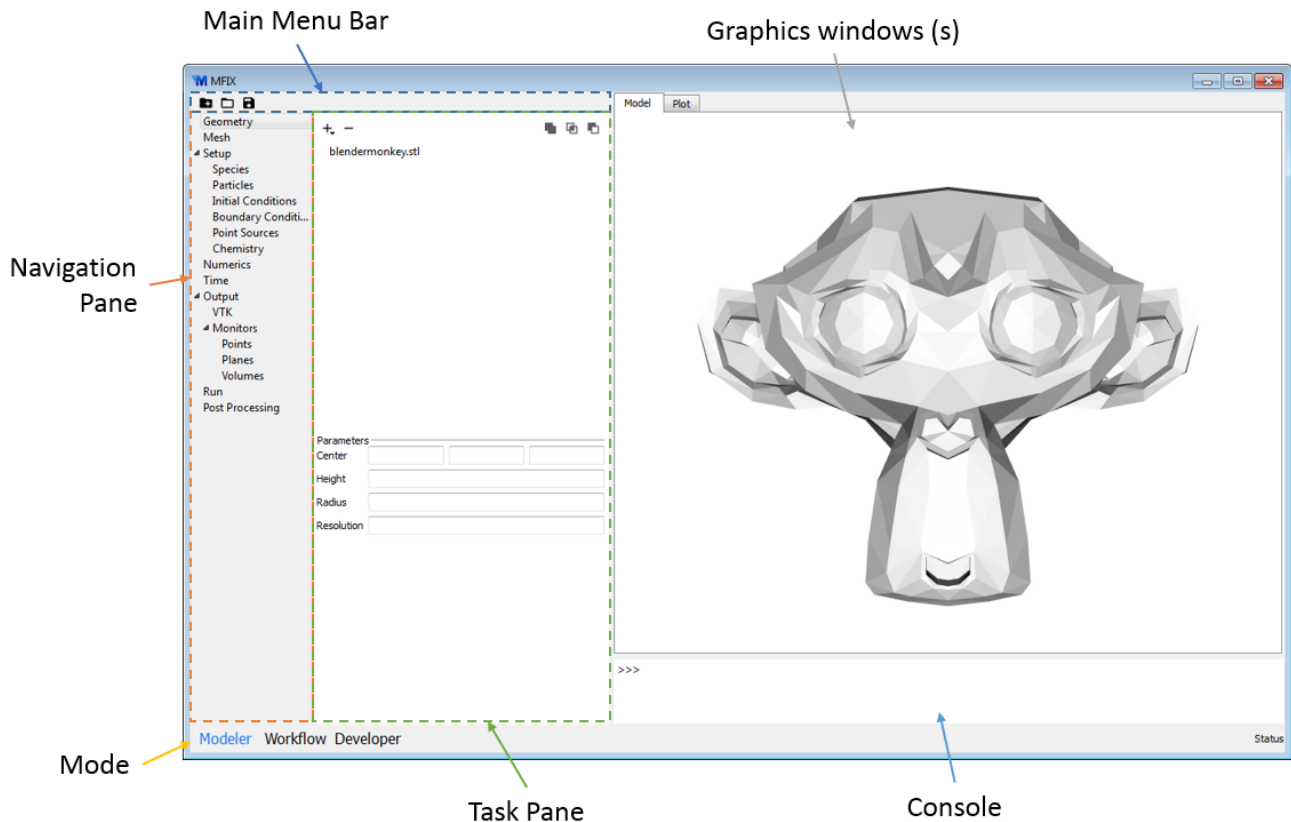


Figure 2: General layout of the Modeler mode

### Navigation Pane:

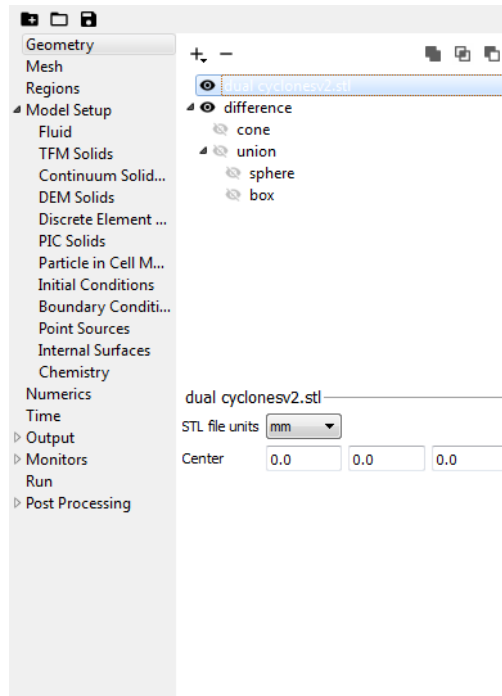
- Geometry
- Mesh
- Regions
- Model Setup
  1. Fluid (*available unless disabled in solver task pane*)
  2. Solids (*only available if TFM/DEM/PIC/Hybrid solver is selected*)
    - TFM (*only available if TFM or Hybrid solver is selected*)
    - DEM (*only available if DEM or Hybrid solver is selected*)
    - PIC (*available only if PIC solver is selected*)
  3. Initial Conditions
  4. Boundary Conditions
  5. Point Sources
  6. Internal Surfaces
  7. Chemistry
- Numerics
- Output
- Monitors
  1. Points
  2. Planes
  3. Volumes
- Run
- Post Processing



1. Export
2. Plugins

### Geometry Task Pane Window: *Load/create geometry*

- Specify stl file(s)
- Specify primitive(s) (box, sphere, cylinder, cone)
- Apply filters
  1. vtkCleanPolyData, vtkFillHolesFilter, vtkTriangleFilter, vtkDecimate, vtkDecimatePro, vtkQuadricDecimation, vtkQuadricClustering
- Perform boolean operations (union, difference, intersect)
- Edit geometry parameters
  1. STL:
    - Select units, scale accordingly
    - Select center, translate accordingly
    - Rotate about x, y, and z axis
  2. Box:
    - Select center, x, y, z lengths
    - Rotate about x, y, and z axis
  3. Sphere
    - Select center, radius
    - Select resolution
    - Rotate about x, y, and z axis
  4. Cylinder
    - Select center, radius, height
    - Select resolution
    - Rotate about x, y, and z axis
  5. Cone
    - Select center, radius, height, direction
    - Select resolution
    - Rotate about x, y, and z axis



*Mockup of geometry task plane.*

**Mesh Task Pane Window:** *Specify/Generate 3D Cartesian mesh*

- Specify domain extents (xmin, xmax, ymin, ymax, zmin, zmax)
- Specify control points (location, cells, stretch)
- Specify remove small cells tolerances
- Specify snap tolerances
- Create the mesh
- Import a mesh

Geometry  
Mesh  
Regions  
Model Setup  
Numerics  
Time  
Output  
Monitors  
Run  
Post Processing

Uniform  
Min  
Max  
Autosize

Cells  
Cell Size

X Control Points

Position	Cells
----------	-------

Y Control Points

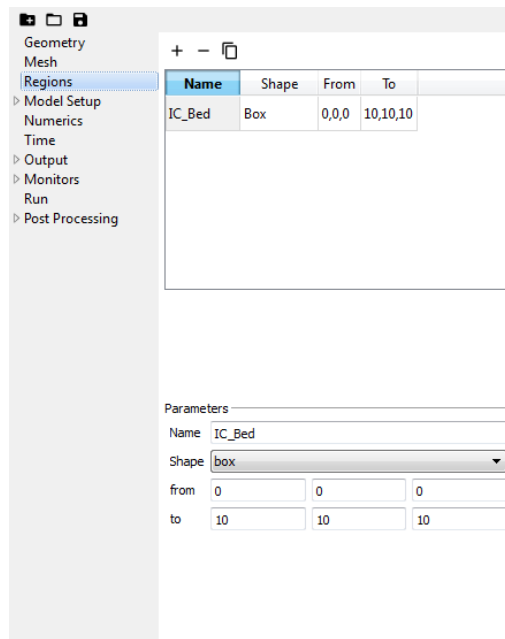
Position	Cells
----------	-------

Z Control Points

Position	Cells
----------	-------

**Regions Task Pane Window:** *Define regions within the domain*

- Specify an alias for easy referencing (e.g., outlet, solids-bed).
- Specify region extents (xmin, xmax, ymin, ymax, zmin, zmax)
- Specify a shape (sphere, cylinder, plane, disk, point)



**Model Setup Task Pane Window:** *Select MFX solver and other conservation equations*

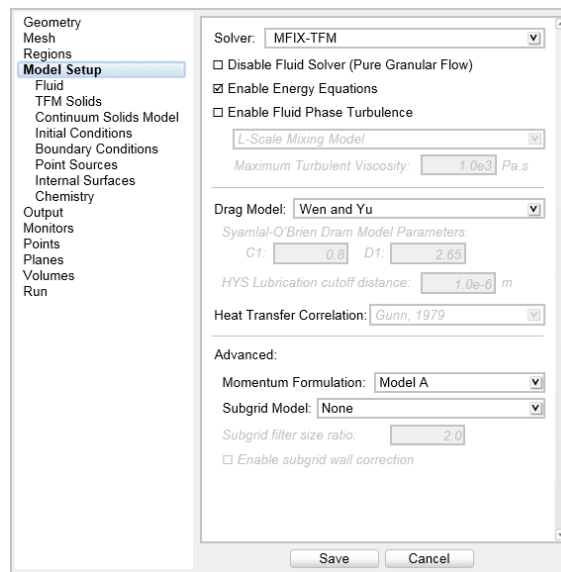
- Select MFX Solver:
  1. Available selections:
    - *Single phase*
      - Selection *disables* 'Solids' task pane menu
      - Selection *disables* 'Continuum Solids Model' task pane menu
      - Selection *disables* 'Discrete Element Model' task pane menu
      - Selection *disables* 'Particle-in-Cell' task pane menu
    - *MFX-TFM*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Continuum Solids Model' task pane menu
    - *MFX-DEM*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Discrete Element Model' task pane menu
    - *MFX-PIC*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Particle-in-Cell' task pane menu
    - *MFX-Hybrid*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Continuum Solids Model' task pane menu
      - Selection *enables* 'Discrete Element Model' task pane menu
- Option to disable the fluid phase
  1. Disables the 'Fluid' task pane menu
  2. Sets keyword RO\_G0 to 0.0
- Option to enable thermal energy equations
  1. This keyword should always be specified in the input deck
  2. Sets keyword ENERGY\_EQ
  3. DEFAULT value of .FALSE.
- Option to enable turbulence
  1. Selection available if fluid phase is enabled

2. Available selections:
  - *None*; [DEFAULT]
  - *Mixing Length*:
    - Selection always available
    - Sets keyword TURBULENCE\_MODEL to MIXING\_LENGTH
    - Requires IC\_L\_SCALE for all IC regions
  - *K-Epsilon*
    - Selection always available
    - Sets keyword TURBULENCE\_MODEL to K\_EPSILON
    - Requires IC\_K\_TURB\_G for all IC regions
    - Requires IC\_E\_TURB\_G for all IC regions
    - Requires BC\_K\_TURB\_G for inflow (MI and PI) BC regions
    - Requires BC\_E\_TURB\_G for inflow (MI and PI) BC regions
- Specify maximum fluid viscosity (not shown in mockup)
  1. Selection available if TURBULENCE\_MODEL  $\neq$  'NONE'
  2. Sets keyword MU\_GMAX
  3. DEFAULT value of 1.0e3 (Pa.s)
- Specify drag model
  1. Selection requires TFM, DEM, or PIC solver
  2. Sets keyword DRAG\_TYPE
  3. Available selections:
    - *SYAM\_OBRIEN* (DEFAULT)
      - Specify model parameter: DRAG\_C1
        - DEFAULT value of 0.8
      - Specify model parameter: DRAG\_D1
        - DEFAULT value of 2.65
    - *BVK*
    - *GIDASPOW*
    - *GIDASPOW\_BLEND*
    - *GIDASPOW\_PCF*
    - *GIDASPOW\_BLEND\_PCF*
    - *HYS*
      - Specify model parameter LAM\_HYS
        - DEFAULT value of 1.0e-6 (meters)
    - *KOCH\_HILL*
    - *KOCH\_HILL\_PCF*
    - *WEN\_YU*
    - *WEN\_YU\_PCF*
    - *USER\_DRAG*
- Specify heat transfer correlation (*requires TFM, DEM, or PIC solver*)
 

*\*This option may be premature as MFI-X is limited in heat HTC's.*
- Specify momentum equation formulation; *Select Model A, Model B; Jackson, Ishii*
- Select sub-grid model:
  1. Selection requirements:
    - Only available with MFI-X-TFM solver
    - DRAG\_TYPE="WEN\_YU"
    - KT\_TYPE="ALGEBRAIC"
    - TURBULENCE\_MODEL  $\neq$  K\_EPSILON
    - BLENDING\_STRESS = NONE
    - FRICTION\_MODEL  $\neq$  SRIVASTAVA
    - (There are more restrictions...)
  2. Sets keyword SUBGRID\_TYPE
  3. Available selections
    - *NONE* (DEFAULT)

- *IGCI*
  - *MILIOLI*
- Specify sub-grid model filter size ratio:
  1. Specification requires SUBGRID\_TYPE  $\neq$  NONE
  2. Sets keyword FILTER\_SIZE\_RATIO
  3. DEFAULT value of 2.0
- Enable sub-grid wall correction model:
  1. Specification requires SUBGRID\_TYPE  $\neq$  NONE
  2. Sets keyword SUBGRID\_WALL
  3. DEFAULT value of FALSE

*Mockup of Task pane for defining the Model Setup.*



**Fluid phase Task Pane Window:** *(unavailable if fluid phase was disabled)*

- Option to rename the phase (e.g, air, gas)
- Option to disable Momentum Equations *(enabled by default)*
  1. Sets keyword: MOMENTUM\_X/Y/Z\_EQ(0)
- Option to enable Species Equations
  1. Sets keyword: SPECIES\_EQ(0)
  2. Species Equations disabled [DEFAULT]
- Option to enable scalar equations
  1. Define the number of scalar equations
  2. Value sums into keyword NSCALAR
  3. Sets keyword PHASE4SCALAR(\*)=0 for total listed scalars
- Select Density Model:
  1. Selection always available
  2. Available selections:
    - *Constant:* [DEFAULT]
      - Selection always available
      - Specify constant gas density, RO\_G0
    - *Ideal gas law:*
      - Selection always available

- Keyword RO\_G0 must be undefined
    - Requires a fluid phase molecular weight
    - Requires temperature field for full domain
  - *UDF*
    - Selection is always available
    - Sets keyword USR\_ROg
    - MFI runtime check verifies UDF was provided
- Select Viscosity Model:
  1. Selection always available
  2. Available selections:
    - *Constant*: [DEFAULT]
      - Selection always available
      - Specify constant gas viscosity, MU\_G0
    - *Sutherland's law*
      - Selection always available
      - Keyword MU\_G0 must be undefined
      - Requires temperature field for full domain
    - *UDF*
      - Selection always available
      - Sets keyword USR\_MUG
      - MFI runtime check verifies UDF was provided
- Select Molecular Weight Model:
  1. Selection always available
  2. Available selections:
    - *Constant*: [DEFAULT]
      - Specification always available
      - Specify constant molecular weight, MW\_AVG
    - *Mixture*:
      - Selection always available
      - Requires molecular weights for all species components
- Select Specific Heat Model:
  1. Selection available only when solving thermal energy equations
  2. Available selections:
    - *Constant*: [DEFAULT]
      - Selection always available
      - Specify constant fluid phase specific heat, C\_PG0
    - *Mixture*:
      - Selection always available
      - Keyword C\_PG0 must be undefined
      - Requires specific heats for all species components
    - *UDF*
      - Selection always available
      - Sets keyword USR\_CPg
      - MFI runtime check verifies UDF was provided
- Select Thermal Conductivity Model:
  1. Selection only available when solving thermal energy equations
  2. Available selections:
    - *Constant*
      - Selection always available
      - Specify constant thermal conductivity, K\_G0
    - *Temperature dependent (air)*: [DEFAULT]
      - Selection always available
      - Keyword K\_G0 must be undefined
    - *UDF*

- Selection always available
  - Set keyword USR\_KG
  - MFIX runtime check verifies UDF was provided
- Select Diffusion Coefficient Model:
  1. Selection only available when solving species equations
  2. Available selections:
    - *Constant*
      - Selection always available
      - Specify a constant diffusion coefficient, DIF\_G0
    - *Dilute Mixture Approximation (air)*; [DEFAULT]
      - Selection always available
      - Keyword DIF\_G0 must be undefined
      - Requires temperature field for full domain
    - *UDF*
      - Selection always available
      - Sets keyword USR\_DIFG
      - MFIX runtime check verifies UDF was provided
- Fluid phase species selection:
  1. Species data required under any of the following conditions:
    - Solving species equations
    - Density model is the ideal gas law with mixture molecular weight model
    - Energy equations are solved with mixture specific heat model
  2. Specification panel operates as a popup window triggered by an Add/Edit button
  3. Summary window provides a list of the species and an overview of some properties

#### Fluid phase Material Database window (popup):

- Select database (BURCAT); later could link in other databases.
- Capability to search selected database for chemical name
- *Import from database* copies the usable information from the database into a new entry in the 'run database'
- *New* creates a new 'blank' species in the 'run database' where the user must supply all the thermochemical data.
- *Delete* removes an entry from the 'run database'

Name	MW	Cp(300K)	Source
O2	32.0	1831.83	BURCAT
CO	28.0	1816.56	BURCAT
CO2	44.0	2319.87	BURCAT
CH4	16.0	2224.08	BURCAT
H2	2.0	1798.34	BURCAT
H2O	18.0	2094.15	BURCAT
Tar	428.3	43.95	User Defined
N2	28.0	1815.46	BURCAT

Source: BURCAT

Species: CH4 ANHARMONIC

Alias: CH4

Molecular weight: 16.0 kg/kmol

Heat of formation: -4649.97 J/kg

Density: kg/m<sup>3</sup>

Specific heat: Polynomial J/(kg.K)

$C_p(T) = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$  J/(kg.K)

Temperature: Low 200.0 High 6000.0

a1: 2.6681E+03 9.9080E+02

**Left:** Mockup of Task pane for defining the fluid phase. Model options toggle between available and unavailable given selections. **Right:** Popup material database window for specifying fluid phase species.

**NOTE:** Generalization of the MFIX solver implementations for specific heat, thermal conductivity, and diffusion coefficient models would naturally lead to more Subtask Panes for each model whereby the user can further define model properties. Presently, these models -especially thermal conductivity and the diffusion coefficient models- are hard coded for specific compositions. This would permit greater modeling flexibility moving forward.

**NOTE:** The gas phase species molecular weights, MW\_G(#) cannot be directly specified. This keyword is not needed because users can edit the molecular weight in the material database popup window.

### Solids Task Pane Window:

- Select Solids model
  1. Sets keyword SOLIDS\_MODEL(#)
  2. Selection locked to Two-Fluid Model (MFIX-TFM) for MFX-TFM solver
  3. Selection locked to Discrete Element Model (MFIX-DEM) for MFX-DEM solver
  4. Selection locked to Multiphase Particle-in-Cell (MFIX-PIC) for MFX-PIC solver
  5. Selections available for MFX-Hybrid solver
    - Two-Fluid Model (MFIX-TFM)
    - Discrete Element Model (MFIX-DEM)
- Option to give the phase a referenceable name (e.g., coal, sand)
  1. Default to Solid-#
- Option to solve Momentum Equations
  1. Selection only available for MFX-TFM solids model
  2. Sets keyword: MOMENTUM\_X/Y/Z\_EQ(#)
  3. Moment equations enabled [DEFAULT]
- Option to enable Species Equations
  1. Sets keyword: SPECIES\_EQ(#)
  2. Species Equations disabled [DEFAULT]
- Option to enable scalar equations
  1. Selection only available for MFX-TFM solids model
  2. Define the number of scalar equations
  3. Value sums into keyword NSCALAR
  4. Sets keyword PHASE4SCALAR(\*)=# for total listed scalars
- Specify Diameter (*required*)
  1. Sets keyword: D\_p0(#)
- Select Solids Density model
  1. Selection requires species equations
  2. Available selections:
    - *Constant*; [DEFAULT]
      - Selection always available
      - Specify a constant solids density, RO\_S0(#)
    - *Variable Solids Density*
      - Selection available with species equations enable
      - Keyword RO\_S0(#) must be undefined
      - Requires material densities for all solids species
      - Requires base composition be specified
      - Requires an inert species be identified
- Select Solids Viscosity Model:
  1. Selection only available for MFX-TFM solids model



2. Available selections:
  - *Continuum Solids Stress Theory* [DEFAULT]
    - Selection always available
    - Keyword MU\_s0 must be undefined
    - Requires selection of viscous solids stress model
    - Requires selection of frictional solids stress model
  - *Constant*
    - Selection always available
    - Specify a constant solids viscosity, MU\_s0(#)
    - Disables selection of viscous solids stress model
    - Disables selection of frictional stress model
  - *UDF*
    - Selection always available
    - Sets keyword USR\_MUS
    - MFI-X runtime check verifies UDF was provided
- Select Molecular Weight Model:
  1. Selection available. Always locked to *Mixture*.
  2. Available selections:
    - *Mixture* [DEFAULT]
      - Selection always available
      - Requires molecular weights for all species components
- Select Specific Heat Model:
  1. Selection available only when solving thermal energy equations
  2. Available selections:
    - *Constant*; [DEFAULT]
      - Selection always available
      - Specify constant solids phase specific heat, C\_PS0(#)
    - *Mixture*:
      - Selection always available
      - Keyword C\_PS0(#) must be undefined
      - Requires specific heats for all species components
    - *UDF*
      - Selection always available
      - Sets keyword USR\_CPS(#)
      - MFI-X runtime check verifies UDF was provided
- Select Thermal Conductivity Model:
  1. Selection only available for MFI-X-TFM solids model
  2. Selection only available when solving thermal energy equations
  3. Available selections:
    - *Constant* [Locked DEFAULT for MFI-X-DEM, MFI-X-PIC]
      - Selection always available
      - Specify constant thermal conductivity, K\_S0(#)
    - *Temperature dependent (ash)*; [DEFAULT]
      - Selection always available
      - Keyword K\_S0(#) must be undefined
    - *UDF*
      - Selection always available
      - Set keyword USR\_KS(#)
      - MFI-X runtime check verifies UDF was provided
- Specify solids phase emissivity
  1. Selection only available for MFI-X-DEM solids model
  2. Specification only available when solving energy equations
  3. Sets keyword DES\_EM(#)
- Solids phase species selection:

1. Species data required under any of the following conditions:
  - Solving species equations
  - Energy equations are solved with mixture specific heat model
2. Specification panel operates as a popup window triggered by an Add/Edit button
3. Summary window provides a list of the species and an overview of some properties
- Baseline (unreacted) composition selection:
  1. Available only for variable solids density model
  2. Select the solids phase species that comprise the initial particle composition
  3. Specify initial mass fractions of the unreacted species,  $X_{s0}(\#, \#)$
  4. Mark one species as an inert material, INERT\_SPECIES( $\#$ )

List the following options under an 'Advanced' section header.

- Option to disable close packing
  1. Selection only available for MFIX-TFM solids model
  2. Sets keyword CLOSE\_PACKED( $\#$ ) = .FALSE.
  3. Disabling close pack triggers a popup warning message.
- Option to include added mass force
  1. Selection only available for MFIX-TFM solids model
  2. Sets keyword ADDED\_MASS and M\_AM= $\#$
  3. Note: Only one phase can have added mass force

The figure consists of two side-by-side screenshots of a software interface for configuring the MFX-TFM solids model. Both screenshots show a sidebar on the left with a tree view containing: Geometry, Mesh, Regions, Model Setup, Fluid, Solids (selected), Continuum Solids Model, Initial Conditions, Boundary Conditions, Point Sources, Internal Surfaces, Chemistry, Output, Monitors, Points, Planes, Volumes, and Run.

**Left Screenshot (Top of task pane):** The 'Solids' panel is active. It features a table with columns: Name, Model, Diameter, and Density. The table contains one entry: 'Sand' with Model 'MFX-TFM', Diameter '800.0e-6', and Density '1200.0'. Below the table, there are several configuration fields:
 

- Model: Two-Fluid Model (MFX-TFM) (dropdown)
- Name: Sand (text field)
- ☒ Solve U-Momentum Equation
- ☒ Solve V-Momentum Equation
- ☒ Solve W-Momentum Equation
- ☐ Enable Species Equations
- ☐ Enable Scalar Equations
- Diameter: 800.0e-6 m (text field)
- Density: Constant (dropdown), 1200.0 kg/m3 (text field)
- Viscosity: Continuum (dropdown), (empty text field) Pa
- Molecular Weight: Mixture (dropdown), (empty text field) kmol/kg
- Specific Heat: Constant (dropdown), 880.0 J/(kg.K) (text field)
- Conductivity: Constant (dropdown), 0.15 W/(m.K) (text field)
- Emissivity: (empty text field)
- Species: (empty text field) with Add/Edit and Delete buttons.

 At the bottom are Save and Cancel buttons.

**Right Screenshot (Bottom of task pane):** This panel shows additional configuration options:
 

- Diameter: 800.0e-6 m (text field)
- Density: Constant (dropdown), 1200.0 kg/m3 (text field)
- Viscosity: Continuum (dropdown), (empty text field) Pa
- Molecular Weight: Mixture (dropdown), (empty text field) kmol/kg
- Specific Heat: Constant (dropdown), 880.0 J/(kg.K) (text field)
- Conductivity: Constant (dropdown), 0.15 W/(m.K) (text field)
- Emissivity: (empty text field)
- Species section: Add/Edit and Delete buttons, followed by a table with columns Name, MW, Cp(300K), and Source.
- Baseline (unreacted) composition section: A table with columns Species, Mass Fraction, and Inert.
- Advanced section:
  - ☐ Disable close pack
  - ☐ Enable added mass force

 At the bottom are Save and Cancel buttons.

Mockup of Task pane for adding non-reacting TFM solids. Clicking the 'Save' button creates the solids phase whereas the 'Cancel' button resets all data fields to the default. In this mockup, solids are listed in a table as they are created. **Left:** Top of the task pane. **Right:** Bottom of task pane.

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
**Solids**  
Discrete Element Model  
Initial Conditions  
Boundary Conditions  
Point Sources  
Internal Surfaces  
Chemistry  
Output  
Monitors  
Points  
Planes  
Volumes  
Run

Solids Add Remove Copy

Name	Model	Diameter	Density
Sand	MFIX-DEM	800.0e-6	1200.0

Model: Discrete Element Model (MFIX-DEM) ▼

Name: Sand

☒ Solve U-Momentum Equation  
☒ Solve V-Momentum Equation  
☒ Solve W-Momentum Equation  
☐ Enable Species Equations  
☐ Enable Scalar Equations

Diameter: 800.0e-6 m  
Density: Constant 1200.0 kg/m3  
Viscosity: Continuum Pa  
Molecular Weight: Mixture kmol/kg  
Specific Heat: Constant 880.0 J/(kg.K)  
Conductivity: Constant 0.15 W/(m.K)  
Emissivity: 0.0

Species Add/Edit Delete

Save Cancel

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
**Solids**  
Discrete Element Model  
Initial Conditions  
Boundary Conditions  
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Chemistry  
Output  
Monitors  
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Planes  
Volumes  
Run

Solids Add Remove Copy

Name	Model	Diameter	Density
Sand	MFIX-DEM	800.0e-6	1200.0

Model: Discrete Element Model (MFIX-DEM) ▼

Name: Sand

☒ Solve U-Momentum Equation  
☒ Solve V-Momentum Equation  
☒ Solve W-Momentum Equation  
☐ Enable Species Equations  
☐ Enable Scalar Equations

Diameter: 800.0e-6 m  
Density: Constant 1200.0 kg/m3  
Viscosity: Continuum Pa  
Molecular Weight: Mixture kmol/kg  
Specific Heat: Constant 880.0 J/(kg.K)  
Conductivity: Constant 0.15 W/(m.K)  
Emissivity: 0.0

Species Add/Edit Delete

Name	MW	Cp(300K)	Source
Baseline (unreacted) composition:			
Species	Mass Fraction	Inert	

Advanced:  
☐ Disable close pack  
☐ Enable added mass force

Save Cancel

Mockup of Task pane for adding non-reacting DEM solids. Clicking the 'Save' button creates the solids phase whereas the 'Cancel' button resets all data fields to the default. In this mockup, solids are listed in a table as they are created. **Left:** Top of the task pane. **Right:** Bottom of task pane

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
**Solids**  
Particle-in-Cell Model  
Initial Conditions  
Boundary Conditions  
Point Sources  
Internal Surfaces  
Chemistry  
Output  
Monitors  
Points  
Planes  
Volumes  
Run

Solids Add Remove Copy

Name	Model	Diameter	Density
Sand	MFIX-PIC	800.0e-6	1200.0

Model: Multiphase Particle-in-Cell (MFIX-PIC) ▼

Name: Sand

☒ Solve U-Momentum Equation  
☒ Solve V-Momentum Equation  
☒ Solve W-Momentum Equation  
☐ Enable Species Equations  
☐ Enable Scalar Equations

Diameter: 800.0e-6 m  
Density: Constant 1200.0 kg/m3  
Viscosity: Continuum Pa  
Molecular Weight: Mixture kmol/kg  
Specific Heat: Constant 880.0 J/(kg.K)  
Conductivity: Constant 0.15 W/(m.K)  
Emissivity:

Species Add/Edit Delete

Save Cancel

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
**Solids**  
Particle-in-Cell Model  
Initial Conditions  
Boundary Conditions  
Point Sources  
Internal Surfaces  
Chemistry  
Output  
Monitors  
Points  
Planes  
Volumes  
Run

Solids Add Remove Copy

Name	Model	Diameter	Density
Sand	MFIX-PIC	800.0e-6	1200.0

Model: Multiphase Particle-in-Cell (MFIX-PIC) ▼

Name: Sand

☒ Solve U-Momentum Equation  
☒ Solve V-Momentum Equation  
☒ Solve W-Momentum Equation  
☐ Enable Species Equations  
☐ Enable Scalar Equations

Diameter: 800.0e-6 m  
Density: Constant 1200.0 kg/m3  
Viscosity: Continuum Pa  
Molecular Weight: Mixture kmol/kg  
Specific Heat: Constant 880.0 J/(kg.K)  
Conductivity: Constant 0.15 W/(m.K)  
Emissivity:

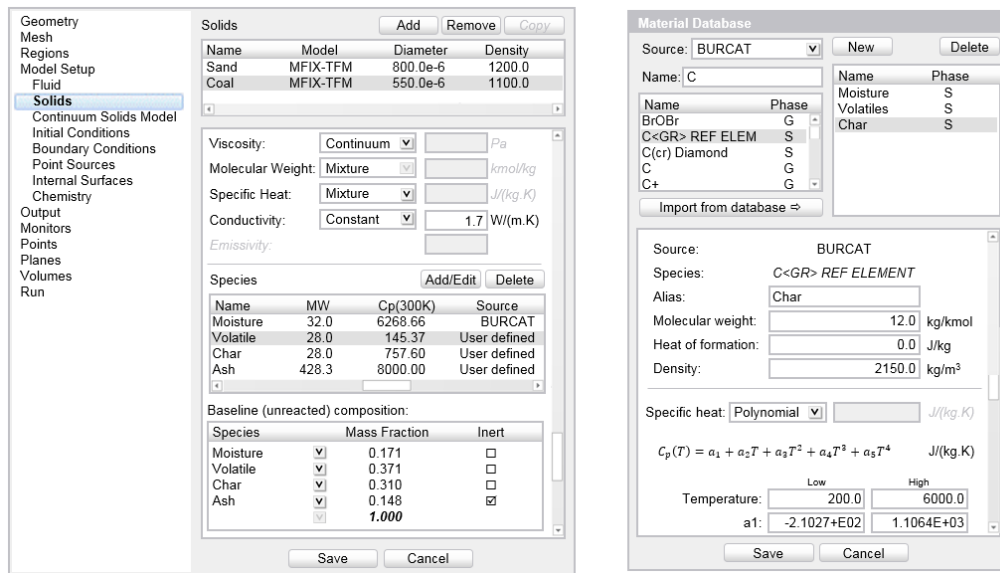
Species Add/Edit Delete

Name	MW	Cp(300K)	Source
Baseline (unreacted) composition:			
Species	Mass Fraction	Inert	

Advanced:  
☐ Disable close pack  
☐ Enable added mass force

Save Cancel

Mockup of Task pane for adding non-reacting PIC solids. Clicking the 'Save' button creates the solids phase whereas the 'Cancel' button resets all data fields to the default. In this mockup, solids are listed in a table as they are created. **Left:** Top of the task pane. **Right:** Bottom of task pane



Mockup of Task pane for adding reacting TFM solids. Note that reactions are consistent across all solids models. **Left:** Bottom of the task pane showing the species information and baseline solids composition. **Right:** Popup material database window for specifying solids phase species.

#### Continuum Solids Model Task Pane Window: (requires TFM solver)

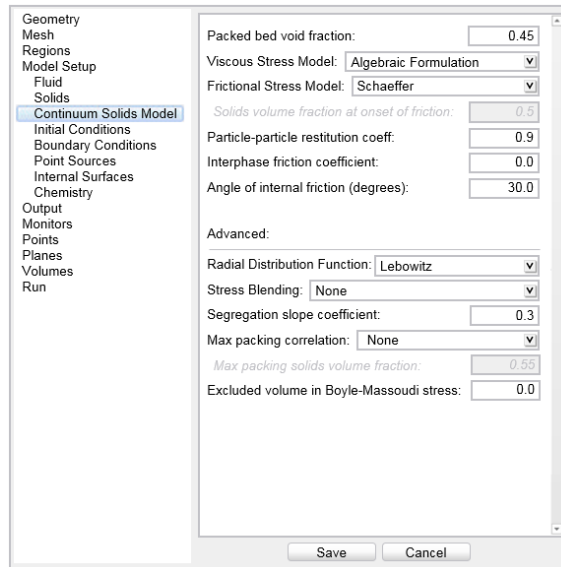
- Specify void fraction at close pack (required)
  1. Sets keyword EP\_STAR
- Select Viscous Stress Model (KTGS):
  1. Selection is unavailable for constant solids viscosity (MU\_S0 defined)
  2. Available selections:
    - Algebraic Formulation [DEFAULT]
      - Selection always available
      - Sets keyword KT\_TYPE to ALGEBRAIC
    - Lun et al, 1984
      - Selection always available
      - Sets keyword KT\_TYPE to LUN\_1984
      - Requires particle-particle restitution coefficient, C\_E
      - If MMAX>1, requires interphase friction coefficient, C\_F
    - Iddir & Arastoopour, 2005
      - Selection always available
      - Sets keyword KT\_TYPE to IA\_NONEP
      - Requires particle-particle restitution coefficient, C\_E
    - Simonin, 1996
      - Selection only available with k-ε turbulence enabled
      - Sets keyword KT\_TYPE to SIMONIN
    - Cao & Ahmadi, 1995
      - Selection only available with k-ε turbulence enabled
      - Sets keyword KT\_TYPE to AHMADI
    - Garzo and Dufty, 1999
      - Selection only available with MMAX=1 (monodisperse)

- Sets keyword KT\_TYPE to GD\_99
  - Requires particle-particle restitution coefficient, C\_E
- Garzo, Tenneti, Subramaniam, Hrenya, 2012
  - Selection only available with MMAX=1 (monodisperse)
  - Sets keyword KT\_TYPE to GTSH
  - Requires particle-particle restitution coefficient, C\_E
- Garzo, Hrenya and Dufty, 2007
  - Selection not available for MMAX > 2
  - Selection not available with added mass force
  - Sets keyword KT\_TYPE to GHD
  - Requires WEN\_YU or HYS drag model
  - Specify coefficient of restitution; R\_p (optional)
- Select Frictional Stress Model
  1. Selection is unavailable for constant solids viscosity (MU\_S0 defined)
  2. Available selections
    - *Schaeffer*
      - Selection always available
      - Sets keyword FRICTION\_MODEL to SCHAEFFER
      - Requires angle of particle-particle friction, PHI
    - *Srivastava and Sundaresan, 2003*
      - Unavailable for Algebraic Formulation viscous stress model
      - Sets keyword FRICTION\_MODEL to SRIVASTAVA
      - Requires angle of particle-particle friction, PHI
      - Requires angle of particle-wall friction, PHI\_W
    - *None*
      - Selection always available
      - Sets keyword FRICTION\_MODEL to NONE
- Specify solids volume fraction at onset of friction
  1. Only available with FRICTION\_MODEL=SRIVASTAVA
  2. Default value of 0.5
  3. Sets keyword EPS\_F\_MIN
- Specify particle-particle restitution coefficient
  1. Specification available only when required
  2. Required for MMAX >=2
  3. Required for viscous stress models except GHD and algebraic formulation
  4. Sets keyword C\_E
- Specify interphase friction coefficient
  1. Specification available only when required
  2. Required for MMAX >= 2
  3. Sets keyword C\_F
- Specify angle of particle-particle friction
  1. Specification available only when required
  2. Required for FRICTION\_MODEL=SCHAEFFER
  3. Required for FRICTION\_MODEL=SRIVASTAVA
  4. Sets keyword PHI

List the following options under an 'Advanced' section header.

- Select radial distribution function
  1. Selection always available
  2. Available selections:
    - Carnahan-Starling
      - Only available for MMAX==1
      - Sets keyword RDF\_TYPE to LEBOWITZ (this is correct)

- *Lebowitz*
    - Only available for  $M_{MAX} > 1$
    - Sets keyword RDF\_TYPE to LEBOWITZ
  - *Mansoori*
    - Only available for  $M_{MAX} > 1$
    - Sets keyword RDF\_TYPE to MANSOORI
  - *Modified Lebowitz*
    - Only available for  $M_{MAX} > 1$
    - Sets keyword RDF\_TYPE to MODIFIED\_LEBOWITZ
  - *Modified Mansoori*
    - Only available for  $M_{MAX} > 1$
    - Sets keyword RDF\_TYPE to MODIFIED\_MANSOORI
- Select stress blending model
  1. Selection only available with FRICTION\_MODEL=SCHAEFFER
  2. Available selections:
    - *None* [DEFAULT]
      - Selection always available
      - Sets keyword BLENDING\_FUNCTION to NONE
    - *Hyperbolic Tangent*
      - Selection always available
      - Sets keyword BLENDING\_FUNCTION to TANH\_BLEND
    - *Sigmoidal*
      - Selection always available
      - Sets keyword BLENDING\_FUNCTION to SIGM\_BLEND
- Specify the segregation slope coefficient
  1. Only available for  $M_{MAX} > 1$  in conjunction with the following viscous stress models: algebraic formulation; Lun, 1984; Simonin, 1996; Ahmadi, 1995
  2. Unavailable with (+other requirements)
  3. Sets keyword SEGREGATION\_SLOPE\_COEFFICIENT
- Select maximum packing correlation
  1. Selection only available with FRICTION\_MODEL=SCHAEFFER and  $M_{MAX} > 1$
  2. Available selections:
    - *Constant* [DEFAULT]
      - Selection always available
      - Sets keyword YU\_STANDIS to false
      - Sets keyword FEDORS\_LANDEL to false
    - *Yu & Standish*
      - Selection only available for  $M_{MAX} = 2$
      - Sets keyword YU\_STANDIS to true
      - Sets keyword FEDORS\_LANDEL to false
    - *Fedors & Landel*
      - Selection always available
      - Sets keyword YU\_STANDIS to false
      - Sets keyword FEDORS\_LANDEL to true
- Specify excluded volume in Boyle-Massoudi stress (*optional*)
  1. Only available with algebraic formulation of viscous stress model
  2. Sets keyword V\_EX



Mockup of Task pane for specifying the continuum solids model parameters.

#### Discrete Element Model Task Pane Window: (requires DEM solver)

- Enable automatic particle generation
  1. Enabled sets keyword GENER\_PART\_CONFIG to true
  2. Disabled enables the user to specify number of entries in particle input file
    - Default value is 0
    - Sets keyword PARTICLES
- Select numerical integration method
  1. Selection always available
  2. Available selections
    - *Euler* [DEFAULT]
      - Selection always available
      - Sets keyword DES\_INTG\_METHOD to 'EULER'
    - *Adams-Bashforth*
      - Selection always available
      - Sets keyword DES\_INTG\_METHOD to 'ADAMS\_BASHFORTH'
- Selection collision model
  1. Selection always available
  2. Available selections
    - *Linear Spring-Dashpot* [DEFAULT]
      - Selection always available
      - Sets keyword DES\_COLL\_MODEL to 'LSD'
    - *Hertzian*
      - Selection always available
      - Sets keyword DES\_COLL\_MODEL to 'HERTZIAN'
- Select gas-solids coupling scheme:
  1. Selection unavailable if fluid model is disabled
  2. Available selections:
    - *One-way Coupled*
      - Selection always available
      - Sets keyword DES\_ONEWAY\_COUPLED true
    - *Fully Coupled* [DEFAULT]

- Selection always available
  - Sets keyword DES\_ONEWAY\_COUPLED false
- Optional to enable explicitly coupled simulation
  1. *Unavailable for GARG\_2012 interpolation*
- Select interpolation framework:
  1. Selection always available
  2. Available selections:
    - *field-to-particle and particle-to-field* [DEFAULT]
      - Sets keyword DES\_INTERP\_ON to true
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to true
    - *field-to-particle only*
      - Sets keyword DES\_INTERP\_ON to true
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to false
    - *particle-to-field only*
      - Sets keyword DES\_INTERP\_ON to false
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to true
    - *no-interpolation*
      - Sets keyword DES\_INTERP\_ON to false
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to false
- Select interpolation scheme:
  1. Selection available except when no-interpolation framework is selected
  2. Available selections:
    - *None* [locked default for no-interpolation framework]
      - Selection always available
      - Sets keyword DES\_INTERP\_SCHEME='NONE'
    - *Garg 2012*
      - Selection not available with explicit coupling enabled
      - Sets keyword DES\_INTERP\_SCHEME='GARG\_2012'
    - *Square DPVM*
      - Selection always available
      - Requires an interpolation width, DES\_INTERP\_WIDTH
      - Sets keyword DES\_INTERP\_SCHEME='SQUARE\_DPVM'
- Define interpolation width (*DPVM only*) (*required*)
  1. Specification only available with SQUARE\_DPVM interpolation scheme
  2. Sets keyword DES\_INTERP\_WIDTH
- Option to enable diffusion of particle data
  1. Selection unavailable with GARG\_2012 interpolation scheme
  2. No keyword is set by this option
  3. Enables the user to specify a diffusion width
    - Sets keyword DES\_DIFFUSE\_WIDTH
- Specify friction coefficient
  1. Specification always required
  2. Sets keyword MEW (MEW\_W)
- Specify normal spring constant
  1. Only available for LSD collision model
  2. Sets keyword KN (KN\_W)
- Specify tangential spring constant factor
  1. Only available for LSD collision model
  2. Sets keyword KT\_FAC (KT\_W\_FAC)
  3. Default values of 2.0/7.0
- Specify tangential damping coefficient factor
  1. Only available for LSD collision model
  2. Sets keyword DES\_ETAT\_FAC (DES\_ETAT\_W\_FAC)
  3. Default values of 0.5 and Specify Young's modulus



- 4. Only available for Hertzian collision model
  - 5. Sets keyword E\_YOUNG (EW\_YOUNG)
- Specify Poisson ratio:
  - 1. Only available for Hertzian collision model
  - 2. Sets keyword V\_POISSON (VW\_POISSON)
- Specify normal restitution coefficient
  - 1. Specification always required
  - 2. Sets keyword DES\_EN\_INPUT (DES\_EN\_WALL\_INPUT)
  - 3. Input given as an upper triangular matrix
- Specify tangential restitution coefficient
  - 1. Specification available for Hertzian collision model
  - 2. Sets keyword DES\_ET\_INPUT (DES\_ET\_WALL\_INPUT)
  - 3. Input given as an upper triangular matrix
- Select cohesion model
  - 1. Selection always available
  - 2. Available selections
    - *None* [DEFAULT]
      - Selection always available
      - Sets keyword USE\_COHESION to false
      - Sets keyword VAN\_DER\_WAALS to false
    - *Van der Waals*
      - Selection always available
      - Sets keyword USE\_COHESION to true
      - Sets keyword VAN\_DER\_WAALS to true
- Specify Hamaker constant
  - 1. Specification only available for Van der Waals cohesion model
  - 2. Sets keyword HAMAKER\_CONSTANT (WALL\_HAMAKER\_CONSTANT)
- Specify outer cutoff;
  - 1. Specification only available for Van der Waals cohesion model
  - 2. Sets keyword VDW\_OUTER\_CUTOFF (WALL\_OUTER\_CUTOFF)
- Specify inner cutoff
  - 1. Specification only available for Van der Waals cohesion model
  - 2. Sets keyword VDW\_INNER\_CUTOFF (WALL\_INNER\_CUTOFF)
- Specify asperities
  - 1. Specification only available for Van der Waals cohesion model
  - 2. Sets keyword ASPERITIES

List the following options under an 'Advanced' section header.

- Select Neighbor Search Method
  - 1. Selection always available
  - 2. Available selection
    - *Grid-based* [DEFAULT]
      - Selection always available
      - Sets keyword DES\_NEIGHBOR\_SEARCH 4
    - *N-Square*
      - Selection always available
      - Sets keyword DES\_NEIGHBOR\_SEARCH 1
- Specify maximum steps between neighbor search
  - 1. Specification always available
  - 2. Sets keyword NEIGHBOR\_SEARCH\_N
- Specify factor defining particle neighborhood
  - 1. Specification always available
  - 2. Sets keyword FACTOR\_RLM

- Specify neighborhood search radius ratio
  1. Specification always available
  2. Sets keyword NEIGHBOR\_SEARCH\_RAD\_RATIO
- Specify search grid partitions (optional)
  1. Specification always available
  2. Sets keyword DESGRIDSEARCH\_IMAX
  3. Sets keyword DESGRIDSEARCH\_JMAX
  4. Sets keyword DESGRIDSEARCH\_KMAX
- Enable user scalar tracking
  1. Selection always available
  2. Does not directly set any keywords
  3. Enables specification of number of user scalars
    - Sets keyword DES\_USR\_VAR\_SIZE
- Define minimum distance for contact conduction (optional)
  1. *Unavailable if not solving energy equations*
- Define fluid lens proportion constant (optional)
  1. *Unavailable if not solving energy equations*

Geometry  
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Run

☒ Enable automatic particle generation  
Data file particle count:   
Integration method: Euler  
Collision Model: Linear spring-dashpot  
Coupling method: Fully coupled  
☒ Enable explicit coupling of interphase quantities  
Interpolation: grid-to-particle and particle-to-grid  
Scheme: Square DPVM Width: 1285.0e-6 m  
☐ Enable mean field diffusion Width:  m

	particle-particle	particle-wall
Friction coefficient:	0.35	0.35
Normal spring constant:	1.0e5	1.0e5 N/m
Spring norm/tang ratio:	0.4	0.4
Damping norm/tang ratio:	0.5	0.5
Young's modulus:	<input type="text"/>	<input type="text"/> Pa
Poisson ratio:	<input type="text"/>	<input type="text"/>

Normal restitution coefficients:	
	Sand Coal
Sand	0.90 0.87
Coal	0.85 0.87
Wall	0.90 0.87

Save Cancel

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
Solids  
**Discrete Element Model**  
Initial Conditions  
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Point Sources  
Internal Surfaces  
Chemistry  
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Planes  
Volumes  
Run

Tangential restitution coefficients:

Cohesion model: None  
Hamaker constant:  particle-particle  particle-wall  
Outer cutoff:  m  
Inner cutoff:  m  
Asperities:  0.0 m

Neighbor search method: Grid based search  
Max steps between neighbor search: 25  
Factor defining particle neighborhood: 1.2  
Distance/diameter triggering search: 1.0  
Search grid partitions (optional):  
IMAX:  JMAX:  KMAX:

☐ Enable user scalar tracking

Minimum conduction distance: 1.0e-6 m  
Fluid lens proportional constant: 0.2

Save Cancel

*Mockup of Task pane for specifying the discrete element model parameters.*

#### **Particle in Cell Model Task Pane Window: (requires PIC solver)**

- Specify void fraction at close pack (required)
  1. Sets keyword EP\_STAR [0.42]
- Define parcel CFL number
  1. Sets keyword CFL\_PIC
  2. DEFAULT value of 0.1
- Select solid stress model
  1. Selection always available
  2. Available selection
    - *Snider, 2001* [DEFAULT]
      - Selection always available
      - Sets keyword MPPIC\_SOLID\_STRESS\_SNIDER=.T.
- Option to enable implicit treatment of drag force
  1. Sets keyword: MPPIC\_PDRAG\_IMPLICIT

- 2. Disabled [DEFAULT]
- Define particle-particle momentum retention
  - 1. Sets keyword MPPIC\_COEFF\_EN1
  - 2. DEFAULT value of 0.4
- Define wall normal momentum retention
  - 1. Sets keyword MPPIC\_COEFF\_EN\_WALL
  - 2. DEFAULT value of 0.3
- Define wall tangential momentum retention
  - 1. Sets keyword MPPIC\_COEFF\_ET\_WALL
  - 2. DEFAULT value of 0.99
- Select gas-solids coupling scheme:
  - 1. Selection unavailable if fluid model is disabled
  - 2. Available selections:
    - One-way Coupled
      - Selection always available
      - Sets keyword DES\_ONEWAY\_COUPLED true
    - Fully Coupled
      - Selection always available
      - Sets keyword DES\_ONEWAY\_COUPLED false
- Select interpolation framework:
  - 1. Selection always available
  - 2. Available selections:
    - *field-to-particle and particle-to-field* [DEFAULT]
      - Sets keyword DES\_INTERP\_ON to true
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to true
    - *field-to-particle only*
      - Sets keyword DES\_INTERP\_ON to true
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to false
    - *particle-to-field only*
      - Sets keyword DES\_INTERP\_ON to false
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to true
    - *no-interpolation*
      - Sets keyword DES\_INTERP\_ON to false
      - Sets keyword DES\_INTERP\_MEAN\_FIELDS to false
- Select interpolation scheme:
  - 1. Selection available except when no-interpolation framework is selected
  - 2. Available selections:
    - *None* [locked default for no-interpolation framework]
      - Selection not available
      - Sets keyword DES\_INTERP\_SCHEME='SQUARE\_DPVM'
    - *Garg 2012*
      - Selection not available with explicit coupling enabled
      - Sets keyword DES\_INTERP\_SCHEME='GARG\_2012'
    - *Square DPVM*
      - Selection always available
      - Requires an interpolation width, DES\_INTERP\_WIDTH
      - Sets keyword DES\_INTERP\_SCHEME='SQUARE\_DPVM'
- Define interpolation width (*DPVM only*) (*required*)
  - 1. Specification only available with SQUARE\_DPVM interpolation scheme
  - 2. Sets keyword DES\_INTERP\_WIDTH
- Define solids stress model parameter: pressure constant
  - 1. Sets keyword PSFAC\_FRIC\_PIC
  - 2. DEFAULT value of 10.0
- Define solids stress model parameter: volume fraction exponent

1. Sets keyword FRIC\_EXP\_PIC
2. DEFAULT value of 3.0
- Define solids stress model parameter: non-singularity factor
  1. Sets keyword FRIC\_NON\_SING\_FAC
  2. DEFAULT value of 1.0E-8

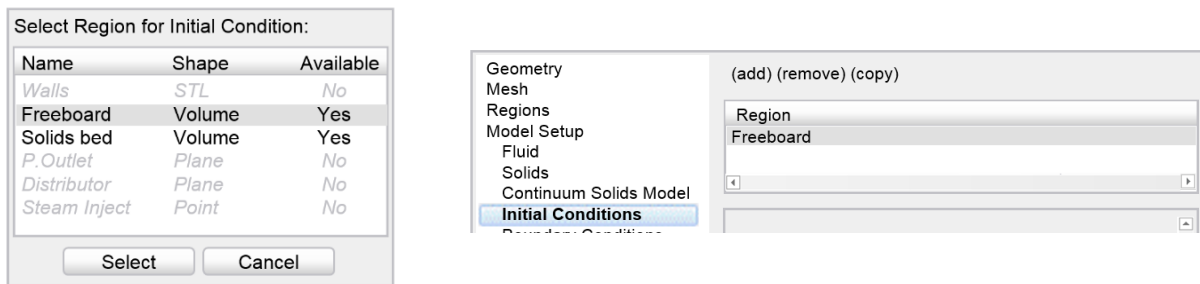
*Mockup of Task pane for specifying the particle in cell model parameters.*

**Initial Conditions Task Pane Window:** This section allows a user to define the initial conditions for the described model. This section relies on regions named in the Regions section.

The top of the task pane is where users define/select IC regions

- Icons to add/remove/duplicate regions are given at the top
- Clicking the 'add' and 'duplicate' buttons triggers a popup window where the user must select the region to apply the initial condition.
  - Users cannot select inapplicable regions.
  - IC regions must be volumes or planes (not points or STLs)
    - Volumes are always valid IC regions
    - XY-Planes are valid IC regions for 2D simulations (NO\_K=.TRUE.)
    - XZ- and YZ Planes are never valid IC regions
  - No region can define more than one initial condition.

*Implementation Idea: Allow the user to select multiple regions in the popup window so that they can define one IC region over multiple regions. Managing the MFI-X IC indices on the back end could get messy, and if so, scrap this idea.*



Tabs group initial condition parameters for phases and additional equations. Tabs are unavailable if no input is required from the user.

- Fluid tab - Unavailable if the fluid phase was disabled.
- Each solid phase will have its own tab. The tab name should be the name of the solid
- Group tab inputs by equation type (e.g., momentum, energy, species). Making the grouped inputs a 'collapsible list' may make navigation easier.

### **Fluid (tab)**

- Define volume fraction
  1. Specification never available
  2. Sets keyword IC\_EP\_G(#)
  3. CALCULATED from  $1.0 - \sum(\text{IC\_EP\_s}(\#, \#))$
  4. GUI should show the result of the calculation.
- Define temperature
  1. Specification always available
  2. Input required for any of the following
    - Fluid density model: Ideal Gas Law
    - Fluid viscosity model: Sutherland's Law
    - Energy equations are solved
  3. Sets keyword IC\_T\_G(#)
  4. DEFAULT value of 293.15
- Define pressure (*optional*)
  1. Specification always available
  2. Sets keyword IC\_P\_g(#)
  3. DEFAULT - no input-
- Define velocity components (*required*)
  1. Specification always available
  2. Sets keywords IC\_U\_G(#), IC\_V\_G(#), IC\_W\_G(#)
  3. DEFAULT value of 0.0
- Select species and set mass fractions (table format)
  1. Specification always available
  2. Sets keyword IC\_X\_G
  3. Input required for species equations
  4. Drop down menu of fluid species
  5. DEFAULT - last defined species has mass fraction of 1.0
  6. Error check: mass fractions must sum to one
- Turbulence: Define mixing length model length scale
  1. Specification only available with Mixing Length turbulence model
  2. Sets keyword IC\_L\_SCALE(#)
  3. DEFAULT value of 1.0
- Turbulence: Define k-ε turbulent kinetic energy

1. Specification only available with K-Epsilon turbulence model
2. Sets keyword IC\_K\_TURB\_G(#)
3. DEFAULT value of 0.0
- Turbulence: Define k-ε turbulent dissipation
  1. Specification only available with K-Epsilon turbulence model
  2. Sets keywords IC\_E\_TURB\_G(#)
  3. DEFAULT value of 0.0
- Advanced: Define radiation coefficient
  1. Specification only available when solving energy equations
  2. Sets keyword IC\_GAMA\_RG(#)
  3. DEFAULT value of 0.0
- Advanced: Define radiation temperature
  1. Specification only available when solving energy equations
  2. Sets keyword IC\_T\_RG(#)
  3. DEFAULT value of 293.15

Geometry  
Mesh  
Regions  
Model Setup  
Fluid  
Solids  
Continuum Solids Model  
**Initial Conditions**  
Boundary Conditions  
Point Sources  
Internal Surfaces  
Chemistry  
Output  
Monitors  
Points  
Planes  
Volumes  
Run

(add) (remove) (copy)

Region  
Freeboard

Fluid Sand Coal Scalar

Volume fraction: 1.0

Temperature: 293.15 K

Pressure: Pa

U-Velocity: 0.0 m/s

V-Velocity: 0.0 m/s

W-Velocity: 0.0 m/s

Species	Mass Fraction
O2	0.23
N2	0.77

Turbulence:

Mixing length model length scale: 0.0 m

k-ε turbulent kinetic energy: 0.0 TBD

k-ε turbulent dissipation: 0.0 TBD

Save Cancel

*Mockup of Task pane for specifying the fluid properties for initial conditions parameters.*

**Solid-# (tab)** - Rename tab to user provided solids name.

- Define volume fraction (required)
  1. Specification always available
  2. Sets keyword IC\_EP\_S(#,#)
  3. DEFAULT value of 0.0
  4. Some input decks may or may not contain IC\_EP\_S keyword:
    - Volume fraction is specified using the solids bulk density
      - $IC\_EP\_S(\#, \#) == IC\_ROP\_S(\#, \#) / IC\_ROs(\#)$
      - Solids density IC\_ROs is determined by the solids density model
        - $IC\_ROs(\#) = RO\_S0(\#)$
        - $IC\_ROs(\#) = --\text{FINISH LATER}--$
    - Volume fraction may be inferred from IC\_EP\_G
      - $IC\_EP\_S(\#, \#) = 1.0 - IC\_EP\_G(\#)$
      - Only valid for one solids phase (MMAX=1)
- Define temperature
  1. Specification always available
  2. Input required when solving energy equations

3. Sets keyword IC\_T\_S(##)
4. DEFAULT value of 293.15
- Define velocity components (*required*)
  1. Specification always available
  2. Sets keywords IC\_U\_S(##), IC\_V\_S(##), IC\_W\_S(##)
  3. DEFAULT value of 0.0
- Define pressure (*optional*)
  1. Specification only available for SOLIDS\_MODEL(#)='TFM'
  2. Sets keyword IC\_P\_STAR(##)
  3. DEFAULT of 0.0
  4. Common to all phases - Warn user if changed.
- Define granular temperature
  1. Specification only available for SOLIDS\_MODEL(#)='TFM' and non-algebraic formulation viscous stress model (see continuous solids model section) or for SOLIDS\_MODEL(#)=DEM' or SOLIDS\_MODEL(#)=PIC'
  2. Sets keyword IC\_THETA\_M(##)
  3. DEFAULT value of 0.0
- Define particles per parcel
  1. Specification only available for SOLIDS\_MODEL(#)=PIC'
  2. Sets keyword IC\_PIC\_CONST\_STATWT(##)
  3. DEFAULT value of 10.0
- Select species and set mass fractions (table format)
  1. Specification always available
  2. Input required for species equations
  3. Drop down menu of solids species
  4. Sets keyword IC\_X\_S(##,##)
  5. DEFAULT - last defined species has mass fraction of 1.0
  6. Error check: mass fractions must sum to one
- Advanced: Option to enable fitting DES particles to region
  1. Option only available for DEM solids
  2. Sets keyword: IC\_DES\_FIT\_TO\_REGION
  3. Disabled [DEFAULT]
- Advanced: Define radiation coefficient
  1. Specification only available when solving energy equations
  2. Sets keyword IC\_GAMA\_RS(##)
  3. DEFAULT value of 0.0
- Advanced: Define radiation temperature
  1. Specification only available when solving energy equations
  2. Sets keyword IC\_T\_RS(##)

## 3. DEFAULT value of 293.15

The image shows a software window titled 'Initial Conditions' with a sidebar on the left containing a tree view of model components: Geometry, Mesh, Regions, Model Setup, Fluid, Solids, Continuum Solids Model, Initial Conditions (selected), Boundary Conditions, Point Sources, Internal Surfaces, Chemistry, Output, Monitors, Points, Planes, Volumes, and Run. The main panel has a tabbed interface with tabs for Fluid, Sand, Coal, and Scalar. The 'Coal' tab is active, showing input fields for Volume fraction (0.23), Temperature (293.15 K), U-Velocity (0.0 m/s), V-Velocity (0.0 m/s), W-Velocity (0.0 m/s), Pressure (optional) (Pa), Granular temperature (0.0), and Particles per parcel. Below these fields is a table for species mass fractions:

Species	Mass Fraction
Char	0.41
Ash	0.59

At the bottom of the panel are 'Save' and 'Cancel' buttons.

*Mockup of Task pane for specifying solids-# initial condition parameters.*

**Scalar (tab)** - Tab only available if scalar equations are solved

- Define initial scalar value
  1. Sets keyword IC\_SCALAR(##)
  2. DEFAULT value of 0.0

The image shows the same software window as above, but with the 'Scalar' tab selected. The 'Coal' tab is now inactive. The main panel shows input fields for 'Scalar-1' (0.0) and 'Scalar-2' (0.0). The 'Save' and 'Cancel' buttons are at the bottom.

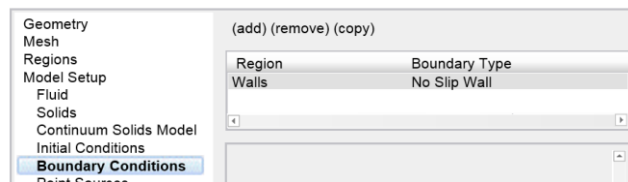
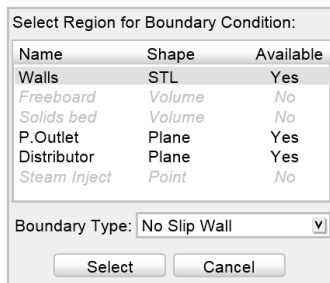
*Mockup of Task pane for specifying the Scalar properties for initial condition regions. Note that this tab should only be available if scalar equations are being solved. Furthermore, the number of scalars requiring input (here 2) comes from the number of scalar equations specified by the user.*

**Boundary Conditions Task Pane Window:** This section allows a user to define the boundary conditions for the described model. This section relies on regions named in the Regions section.



The top of the task pane is where users define/select BC regions

- Icons to add/remove/duplicate boundary conditions are given at the top
- Clicking the 'add' and 'duplicate' buttons triggers a popup window where the user must select a region to apply the boundary condition.
  - Users cannot select inapplicable regions.
  - BC regions must be planes, volumes, or STLs (not points)
  - No region can define more than one boundary condition.
- Select boundary type
  - Selection is required
  - Available selections:
    - *Mass Inflow*
      - Plane regions set keyword BC\_TYPE(#) to 'MI'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_MI'
      - Not available for volume regions
    - *Pressure Outflow*
      - Plane regions set keyword BC\_TYPE(#) to 'PO'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_PO'
      - Not available for volume regions
    - *No Slip Wall*
      - Volume and plane regions set keyword BC\_TYPE(#) to 'NSW'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_NSW'
    - *Free Slip Wall*
      - Volume and plane regions set keyword BC\_TYPE(#) to 'FSW'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_FSW'
    - *Partial Slip Wall*
      - Volume and plane regions set keyword BC\_TYPE(#) to 'PSW'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_PSW'
    - *Pressure Inflow*
      - Plane regions set keyword BC\_TYPE(#) to 'PI'
      - Not available for volume regions
      - Not available for STL regions
    - *Mass Outflow*
      - Plane regions set keyword BC\_TYPE(#) to 'MO'
      - STL regions set keyword BC\_TYPE(#) to 'CG\_MO'
      - Not available for volume regions
    - *Cyclic*
      - No region to select
  - Specification always available
  - DEFAULT - No slip wall
  - Error check: mass fractions must sum to one



Tabs group boundary condition parameters for phases and additional equations. Tabs are unavailable if no input is required from the user.

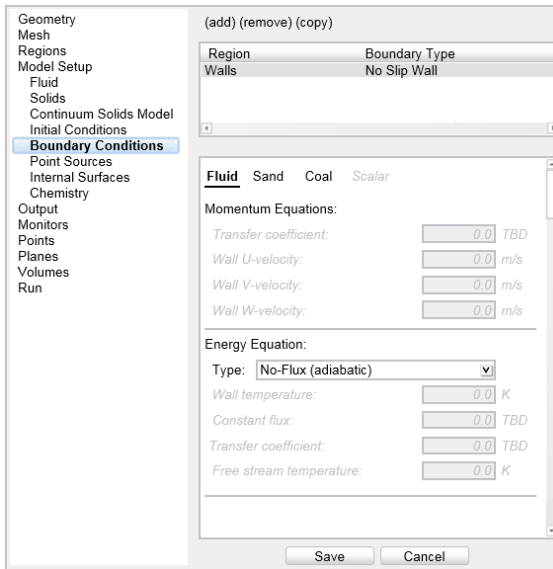
- Fluid tab - Unavailable if the fluid phase was disabled.
- Each solid phase will have its own tab. The tab name should be the name of the solid
- Group tab inputs by equation type (e.g., momentum, energy, species). Making the grouped inputs a 'collapsible list' may make navigation easier.

### **Subtask Pane Tab for Wall type (NSW, FSW, PSW, CG NSW, CG FSW, CG PSW) Boundary Condition Regions**

#### **Fluid (tab)**

- Define transfer coefficient
  1. Specification only available with PSW
  2. Sets keyword BC\_HW\_G(#)
  3. DEFAULT value of 0.0
- Define Wall U-velocity
  1. Specification only available with PSW
  2. Sets keyword BC\_UW\_G(#)
  3. DEFAULT value of 0.0
- Define Wall V-velocity
  1. Specification only available with PSW
  2. Sets keyword BC\_VW\_G(#)
  3. DEFAULT value of 0.0
- Define Wall W-velocity
  1. Specification only available with PSW
  2. Sets keyword BC\_WW\_G(#)
  3. DEFAULT value of 0.0
- Select energy equation boundary type:
  1. Selection only available when solving energy equations
  2. Available selections:
    - *No-Flux (adiabatic)* [DEFAULT]
      - Sets keyword BC\_HW\_T\_G(#) to 0.0
      - Sets keyword BC\_C\_T\_G(#) to 0.0
      - Sets keyword BC\_TW\_G(#) to UNDEFINED
    - *Specified Temperature*
      - Sets keyword BC\_HW\_T\_G(#) to UNDEFINED
      - Sets keyword BC\_C\_T\_G(#) to 0.0
      - Requires BC\_TW\_G(#)
    - *Specified Flux*
      - Sets keyword BC\_HW\_T\_G(#) to 0.0
      - Requires BC\_C\_T\_G(#)
      - Sets keyword BC\_TW\_G(#) to UNDEFINED
    - *Convective Flux*
      - Requires BC\_HW\_T\_G(#)
      - Sets keyword BC\_C\_T\_G(#) to 0.0
      - Requires BC\_TW\_G(#)
- Define wall temperature
  1. Specification only available with 'Specified Temperature' BC type
  2. Sets keyword BC\_TW\_G(#)
  3. DEFAULT value of 293.15
- Define constant flux

1. Specification only available with '*Specified Flux*' BC type
2. Sets keyword BC\_C\_T\_G(#)
3. DEFAULT value of 0.0
- Define transfer coefficient
  1. Specification only available with '*Convective Flux*' BC type
  2. Sets keyword BC\_HW\_T\_G(#)
  3. DEFAULT value of 0.0
- Define free stream temperature
  1. Specification only available with '*Convective Flux*' BC type
  2. Sets keyword BC\_TW\_G(#)
  3. DEFAULT value of 0.0
- Select species equation boundary type:
  1. Selection only available when solving species equations
  2. Available selections:
    - *No-Flux* [DEFAULT]
      - Sets keyword BC\_HW\_X\_G(#) to 0.0
      - Sets keyword BC\_C\_X\_G(#) to 0.0
      - Sets keyword BC\_XW\_G(#) to UNDEFINED
    - *Specified Mass Fraction*
      - Sets keyword BC\_HW\_X\_G(#) to UNDEFINED
      - Sets keyword BC\_C\_X\_G(#) to 0.0
      - Requires BC\_XW\_G(#)
    - *Specified Flux*
      - Sets keyword BC\_HW\_X\_G(#) to 0.0
      - Requires BC\_C\_X\_G(#)
      - Sets keyword BC\_XW\_G(#) to UNDEFINED
    - *Convective Flux*
      - Requires BC\_HW\_X\_G(#)
      - Sets keyword BC\_C\_X\_G(#) to 0.0
      - Requires BC\_XW\_G(#)
- Define wall mass fraction
  1. Specification only available with '*Specified Mass Fraction*' BC type
  2. Sets keyword BC\_XW\_G(#)
  3. DEFAULT value of 0.0
- Define constant flux
  1. Specification only available with '*Specified Flux*' BC type
  2. Sets keyword BC\_C\_X\_G(#)
  3. DEFAULT value of 0.0
- Define transfer coefficient
  1. Specification only available with '*Convective Flux*' BC type
  2. Sets keyword BC\_HW\_X\_G(#)
  3. DEFAULT value of 0.0
- Define free stream mass fraction
  1. Specification only available with '*Convective Flux*' BC type
  2. Sets keyword BC\_XW\_G(#)
  3. DEFAULT value of 0.0



*Mockup of Task pane for specifying the Fluid properties for WALL boundary condition regions.*

**Comment on Solids Wall BCs:** Most of the solids wall BCs are only needed for TFM solids. PIC does not support ANY of the wall BC specifications. DEM only supports keywords associated with the energy equations.

**Solids-# (tab)** - (Replace with phase name defined by the user)

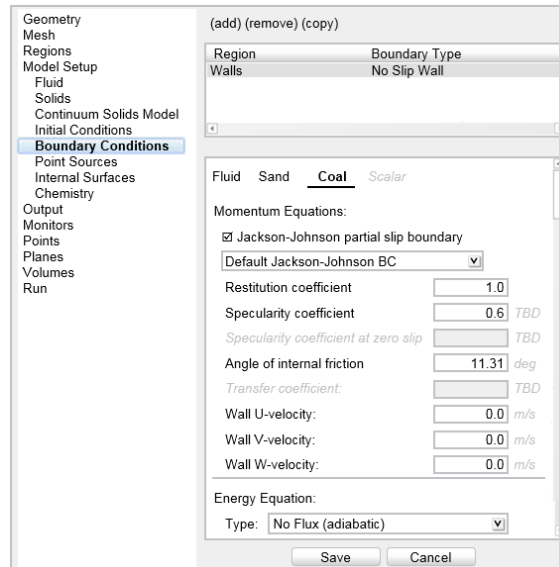
- Enable Jackson-Johnson partial slip boundary
  1. Disabled for DEM and PIC solids
  2. Disabled (0.0) for CARTESIAN\_GRID = .TRUE.
  3. Disabled (0.0) for KT\_TYPE = 'ALGEBRAIC'
  4. Disabled (0.0) for KT\_TYPE = 'GHD\_2007'
  5. Sets keyword BC\_JJ\_PS(#)
  6. DEFAULT value of 1.0 when not disabled
- Select type of Jackson and Johnson BC:
  1. Disabled for DEM and PIC solids
  2. Selection only available BC\_JJ\_PS(#) = 1.0
  3. Available selections:
    - *Default Jackson-Johnson BC [DEFAULT]*
      - Sets keyword BC\_JJ\_M to .FALSE.
      - Sets keyword JENKINS to .FALSE.
    - *Variable specular coefficient*
      - Sets keyword BC\_JJ\_M to .TRUE.
      - Sets keyword JENKINS to .FALSE.
    - *Jenkins small frictional boundary*
      - Sets keyword BC\_JJ\_M to .FALSE.
      - Sets keyword JENKINS to .TRUE.
- Define restitution coefficient
  1. Disabled for DEM and PIC solids
  2. Specification only available with BC\_JJ\_PS(#) = 1.0
  3. Sets keyword E\_W
  4. DEFAULT value of 1.0
  5. Required when available

- Define specular coefficient
  1. Disabled for DEM and PIC solids
  2. Specification only available with BC\_JJ\_PS(#)=1.0 and JENKINS=.FALSE.
  3. Sets keyword PHIP
  4. DEFAULT value of 0.6
  5. Required when available
- Define specular coefficient at zero slip
  1. Disabled for DEM and PIC solids
  2. Specification only available with BC\_JJ\_PS(#)=1.0 and BC\_JJ\_M=.TRUE.
  3. Sets keyword PHIP0
  4. DEFAULT -blank-
  5. Optional when available
- Define angle of internal friction
  1. Disabled for DEM and PIC solids
  2. Sets keyword PHI\_W
  3. Specification only available with BC\_JJ\_PS(#)=1.0 and (JENKINS=.TRUE. FRICION\_MODEL=SRIVASTAVA)
  4. DEFAULT value of 11.31
  5. Required when available
- Define transfer coefficient
  1. Disabled for DEM and PIC solids
  2. Specification only available with PSW
  3. Sets keyword BC\_HW\_S(,#)
  4. DEFAULT value of 0.0
- Define Wall U-velocity
  1. Disabled for DEM and PIC solids
  2. Specification only available with PSW or BC\_JJ\_PS(#)=1.0
  3. Sets keyword BC\_UW\_S(,#)
  4. DEFAULT value of 0.0
- Define Wall V-velocity
  1. Disabled for DEM and PIC solids
  2. Specification only available with PSW or BC\_JJ\_PS(#)=1.0
  3. Sets keyword BC\_VW\_S(,#)
  4. DEFAULT value of 0.0
- Define Wall W-velocity
  1. Disabled for DEM and PIC solids
  2. Specification only available with PSW or BC\_JJ\_PS(#)=1.0
  3. Sets keyword BC\_WW\_S(,#)
  4. DEFAULT value of 0.0
- Select energy equation boundary type:
  1. Disabled for PIC solids
  2. Selection only available when solving energy equations
  3. Available selections:
    - *No-Flux (adiabatic)* [DEFAULT]
      - Sets keyword BC\_HW\_T\_S(,#) to 0.0
      - Sets keyword BC\_C\_T\_S(,#) to 0.0
      - Sets keyword BC\_TW\_S(,#) to UNDEFINED
    - *Specified Temperature*
      - Sets keyword BC\_HW\_T\_S(,#) to UNDEFINED
      - Sets keyword BC\_C\_T\_S(,#) to 0.0
      - Requires BC\_TW\_S(,#)
    - *Specified Flux*
      - Sets keyword BC\_HW\_T\_S(,#) to 0.0
      - Requires BC\_C\_T\_S(,#)

- Sets keyword BC\_TW\_S(#,#) to UNDEFINED
  - *Convective Flux*
    - Disabled for DEM and PIC solids
    - Requires BC\_HW\_T\_S(#,#)
    - Sets keyword BC\_C\_T\_S(#,#) to 0.0
    - Requires BC\_TW\_S(#,#)
- Define wall temperature
  1. Disabled for PIC solids
  2. Specification only available with '*Specified Temperature*' BC type
  3. Sets keyword BC\_TW\_S(#,#)
  4. DEFAULT value of 293.15
- Define constant flux
  1. Disabled for PIC solids
  2. Specification only available with '*Specified Flux*' BC type
  3. Sets keyword BC\_C\_T\_S(#,#)
  4. DEFAULT value of 0.0
- Define transfer coefficient
  1. Disabled for PIC solids
  2. Specification only available with '*Convective Flux*' BC type
  3. Sets keyword BC\_HW\_T\_S(#,#)
  4. DEFAULT value of 0.0
- Define free stream temperature
  1. Disabled for PIC solids
  2. Specification only available with '*Convective Flux*' BC type
  3. Sets keyword BC\_TW\_S(#,#)
  4. DEFAULT value of 0.0
- Select granular energy equation boundary type:
  1. Disabled for DEM and PIC solids
  2. Selection only available with BC\_JJ\_PS(#)=0.0 and KT\_TYPE != 'ALGEBRAIC'
  3. Available selections:
    - *No-Flux* [DEFAULT]
      - Sets keyword BC\_HW\_THETA\_M(#,#) to 0.0
      - Sets keyword BC\_C\_THETA\_M(#,#) to 0.0
      - Sets keyword BC\_THETA\_W\_M(#,#) to UNDEFINED
    - *Specified Temperature*
      - Sets keyword BC\_HW\_THETA\_M(#,#) to UNDEFINED
      - Sets keyword BC\_C\_THETA\_M(#,#) to 0.0
      - Requires BC\_THETA\_W\_M(#,#)
    - *Specified Flux*
      - Sets keyword BC\_HW\_THETA\_M(#,#) to 0.0
      - Requires BC\_C\_THETA\_M(#)
      - Sets keyword BC\_THETA\_W\_M(#,#) to UNDEFINED
- Define granular temperature
  1. Disabled for DEM and PIC solids
  2. Specification only available with '*Specified Temperature*' BC type
  3. Sets keyword BC\_THETA\_W\_M(#,#)
  4. DEFAULT value of 0.0
- Define constant flux
  1. Disabled for DEM and PIC solids
  2. Specification only available with '*Specified Flux*' BC type
  3. Sets keyword BC\_C\_THETA\_M(#,#)
  4. DEFAULT value of 0.0

**When solving solids species equations:**

- Set keyword BC\_HW\_X\_S(#,#,#) to 0.0
- Set keyword BC\_C\_X\_S(#,#,#) to 0.0
- Set keyword BC\_XW\_S(#,#,#) to UNDEFINED

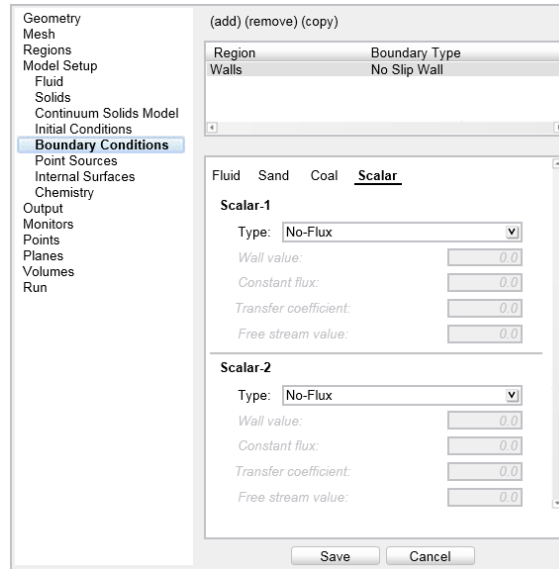


Mockup of Task pane for specifying the Solid-# properties for WALL boundary condition regions.

**Scalar (tab)** - Tab only available if scalar equations are solved

- Select scalar boundary type:
  1. Available selections:
    - *No-Flux* [DEFAULT]
      - Sets keyword BC\_HW\_SCALAR(#,#) to 0.0
      - Sets keyword BC\_C\_SCALAR(#,#) to 0.0
      - Sets keyword BC\_SCALARW(#,#) to UNDEFINED
    - *Specified Temperature*
      - Sets keyword BC\_HW\_SCALAR(#,#) to UNDEFINED
      - Sets keyword BC\_C\_SCALAR(#,#) to 0.0
      - Requires BC\_SCALARW(#,#)
    - *Specified Flux*
      - Sets keyword BC\_HW\_T\_S(#,#) to 0.0
      - Requires BC\_C\_SCALAR(#)
      - Sets keyword BC\_SCALARW(#,#) to UNDEFINED
    - *Convective Flux*
      - Requires BC\_HW\_T\_S(#,#)
      - Sets keyword BC\_C\_SCALAR(#,#) to 0.0
      - Requires BC\_SCALARW(#,#)
- Define wall temperature
  1. Specification only available with '*Specified Temperature*' BC type
  2. Sets keyword BC\_SCALARW(#,#)
  3. DEFAULT value of 0.0
- Define constant flux
  1. Specification only available with '*Specified Flux*' BC type
  2. Sets keyword BC\_C\_SCALAR(#,#)
  3. DEFAULT value of 0.0
- Define transfer coefficient
  1. Specification only available with '*Convective Flux*' BC type

2. Sets keyword BC\_HW\_SCALAR(##)
3. DEFAULT value of 0.0
- Define free stream temperature
  1. Specification only available with 'Convective Flux' BC type
  2. Sets keyword BC\_SCALARW(##)
  3. DEFAULT value of 0.0



Mockup of Task pane for specifying the Scalar properties for WALL boundary condition regions. Note that this tab should only be available if scalar equations are being solved. Furthermore, the number of scalars requiring input (here 2) comes from the number of scalar equations specified by the user.

### **Subtask Pane Tab for INFLOW type (MI, PI, CG MI) Boundary Condition Regions**

#### **Fluid (tab)**

- Define volume fraction
  1. Specification always available
  2. Sets keyword BC\_EP\_G(##)
    - DEFAULT value of 1.0 for MI and CG MI; leave [UNDEFINED] for PI
    - Error Check: For MI and CG MI,  $BC\_EP\_G(\#) + BC\_EP\_S(\#,.) = 1.0$
    - Error Check: For PI - either all are defined and sum to 1, or all are undefined
- Define inflow properties: Mass inflow specification changes based on the BC\_TYPE and Region orientation (e.g., XZ-Plane)
  1. For BC\_TYPE='MI' and XZ-Plane region
    - Select mass inflow specification type:
      - Available selections:
      - Y-Axial Velocity (m/s) [DEFAULT]
        - Sets keyword BC\_V\_G(##)
        - DEFAULT value of 0.0
      - Volumetric Flowrate (m<sup>3</sup>/s)
        - Sets keyword BC\_VOLFLOW\_G(##)
        - DEFAULT value of 0.0
      - Mass Flowrate (kg/s)



- Sets keyword BC\_MASSFLOW\_G(#)
    - DEFAULT value of 0.0
  - Define Tangential Velocities:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_G(#)
      - DEFAULT value of 0.0
    - Define Z-Axial Velocity
      - Sets keyword BC\_W\_G(#)
      - DEFAULT value of 0.0
- 2. For BC TYPE='MI' and YZ-Plane region**
- Select mass inflow specification type:
    - Available selections:
    - *X-Axial Velocity (m/s)* [DEFAULT]
      - Sets keyword BC\_U\_G(#)
      - DEFAULT value of 0.0
    - *Volumetric Flowrate (m<sup>3</sup>/s)*
      - Sets keyword BC\_VOLFLOW\_G(#)
      - DEFAULT value of 0.0
    - *Mass Flowrate (kg/s)*
      - Sets keyword BC\_MASSFLOW\_G(#)
      - DEFAULT value of 0.0
  - Define Tangential Velocities:
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_G(#)
      - DEFAULT value of 0.0
    - Define Z-Axial Velocity
      - Sets keyword BC\_W\_G(#)
      - DEFAULT value of 0.0
- 3. For BC TYPE='MI' and XY-Plane region**
- Select mass inflow specification type:
    - Available selections:
    - *Z-Axial Velocity (m/s)* [DEFAULT]
      - Sets keyword BC\_W\_G(#)
      - DEFAULT value of 0.0
    - *Volumetric Flowrate (m<sup>3</sup>/s)*
      - Sets keyword BC\_VOLFLOW\_G(#)
      - DEFAULT value of 0.0
    - *Mass Flowrate (kg/s)*
      - Sets keyword BC\_MASSFLOW\_G(#)
      - DEFAULT value of 0.0
  - Define Tangential Velocities:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_G(#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_G(#)
      - DEFAULT value of 0.0
- 4. For BC TYPE='CG MI' or 'PI'**
- Specify all velocity components:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_G(#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_G(#)

- DEFAULT value of 0.0
- Define Z-Axial Velocity
  - Sets keyword BC\_W\_G(#)
  - DEFAULT value of 0.0
- Define temperature
  1. Specification always available
  2. Input required for any of the following
    - Fluid density model: Ideal Gas Law
    - Fluid viscosity model: Sutherland's Law
    - Energy equations are solved
  3. Sets keyword BC\_T\_G(#)
  4. DEFAULT value of 293.15
- Define pressure
  1. Specification always available
  2. Input required when combining ideal gas law and specified mass inflow rate
  3. Input required for BC\_TYPE = PI
  4. Sets keyword BC\_P\_G(#)
  5. DEFAULT 101.325d3
- Select species and set mass fractions (table format)
  1. Specification always available
  2. Input required for species equations
  3. Drop down menu of fluid species
  4. Sets keyword BC\_X\_G(,#)
  5. DEFAULT - last defined species has mass fraction of 1.0
  6. Error check: mass fractions must sum to one
- Turbulence: Define k-ε turbulent kinetic energy
  1. Specification only available with K-Epsilon turbulence model
  2. Sets keyword BC\_K\_TURB\_G(#)
  3. DEFAULT value of 0.0
- Turbulence: Define k-ε turbulent dissipation
  1. Specification only available with K-Epsilon turbulence model
  2. Sets keywords BC\_E\_TURB\_G(#)
  3. DEFAULT value of 0.0

Geometry Mesh Regions Model Setup Fluid Solids Continuum Solids Model Initial Conditions <b>Boundary Conditions</b> Point Sources Internal Surfaces Chemistry Output Monitors Points Planes Volumes Run	(add) (remove) (copy) <table border="1"> <thead> <tr> <th>Region</th> <th>Boundary Type</th> </tr> </thead> <tbody> <tr> <td>Walls</td> <td>No Slip Wall</td> </tr> <tr> <td>Distributor</td> <td>Mass Inflow</td> </tr> </tbody> </table> <div> <div>Fluid</div> <div>Sand</div> <div>Coal</div> <div>Scalar</div> </div> Volume Fraction: <input type="text" value="0.98"/> Y-Axial Velocity: <input type="text" value="0.0"/> m/s Tangential Velocity Components: X-Axial Velocity: <input type="text" value="0.0"/> m/s Z-Axial Velocity: <input type="text" value="0.0"/> m/s Pressure: <input type="text" value="0.0"/> Pa Temperature: <input type="text" value="293.15"/> K <table border="1"> <thead> <tr> <th>Species</th> <th>Mass Fraction</th> </tr> </thead> <tbody> <tr> <td>O2 <input checked="" type="checkbox"/></td> <td>0.23</td> </tr> <tr> <td>N2 <input checked="" type="checkbox"/></td> <td>0.77</td> </tr> </tbody> </table> Turbulence: k-ε turbulent kinetic energy: <input type="text" value="0.0"/> TBD k-ε turbulent dissipation: <input type="text" value="0.0"/> TBD	Region	Boundary Type	Walls	No Slip Wall	Distributor	Mass Inflow	Species	Mass Fraction	O2 <input checked="" type="checkbox"/>	0.23	N2 <input checked="" type="checkbox"/>	0.77
Region	Boundary Type												
Walls	No Slip Wall												
Distributor	Mass Inflow												
Species	Mass Fraction												
O2 <input checked="" type="checkbox"/>	0.23												
N2 <input checked="" type="checkbox"/>	0.77												

Mockup of Task pane for specifying the Fluid properties for MI, boundary condition regions.

**Solid-# (tab)** - Rename tab to user provided solids name.

- Define volume fraction
  1. Specification always available
  2. Sets keyword BC\_EP\_S(#,#)
    - DEFAULT value of 1.0 - (sum of previous tabs) for MI and CG\_MI; leave [UNDEFINED] for PI
    - Error Check: For MI and CG\_MI,  $BC\_EP\_G(\#) + BC\_EP\_S(\#,.) = 1.0$
    - Error Check: For PI - either all are defined and sum to 1, or all are undefined
    - Some input decks may or may not contain BC\_EP\_S keyword:
      - Volume fraction is specified using the solids bulk density
        - $BC\_EP\_S(\#,.) = BC\_ROP\_S(\#,.) / BC\_ROs(\#)$
        - Solids density BC\_ROs is determined by solids density model
          - $BC\_ROs(\#) = RO\_S0(\#)$
          - $BC\_ROs(\#) = -- FINISH LATER --$
      - Volume fraction may be inferred from BC\_EP\_G
        - $BC\_EP\_S(\#,.) = 1.0 - BC\_EP\_G(\#)$
        - Only valid for one solids phase (MMAX=1)
- Define inflow properties: *Mass inflow specification changes based on the BC\_TYPE and Region orientation (e.g., XZ-Plane)*
  1. **For BC\_TYPE='MI' and XZ-Plane region**
    - Select mass inflow specification type:
      - Available selections:
      - *Y-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_V\_S(#,#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_S(#,#)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_S(#,#)
        - DEFAULT value of 0.0
    - Define Tangential Velocities:
      - Define X-Axial Velocity
        - Sets keyword BC\_U\_S(#,#)
        - DEFAULT value of 0.0
      - Define Z-Axial Velocity
        - Sets keyword BC\_W\_S(#,#)
        - DEFAULT value of 0.0
  2. **For BC\_TYPE='MI' and YZ-Plane region**
    - Select mass inflow specification type:
      - Available selections:
      - *X-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_U\_S(#,#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_S(#,#)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_S(#, #)

- DEFAULT value of 0.0
- Define Tangential Velocities:
  - Define Y-Axial Velocity
    - Sets keyword BC\_V\_S(#,#)
    - DEFAULT value of 0.0
  - Define Z-Axial Velocity
    - Sets keyword BC\_W\_S(#,#)
    - DEFAULT value of 0.0
- 3. **For BC TYPE='MI' and XY-Plane region**
  - Select mass inflow specification type:
    - Available selections:
    - Z-Axial Velocity (m/s) [DEFAULT]
      - Sets keyword BC\_W\_S(#,#)
      - DEFAULT value of 0.0
    - Volumetric Flowrate (m<sup>3</sup>/s)
      - Sets keyword BC\_VOLFLOW\_S(#,#)
      - DEFAULT value of 0.0
    - Mass Flowrate (kg/s)
      - Sets keyword BC\_MASSFLOW\_S(#,#)
      - DEFAULT value of 0.0
  - Define Tangential Velocities:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_S(#,#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_S(#,#)
      - DEFAULT value of 0.0
- 4. **For BC TYPE='CG MI' or 'PI'**
  - Specify all velocity components:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_S(#,#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_S(#,#)
      - DEFAULT value of 0.0
    - Define Z-Axial Velocity
      - Sets keyword BC\_W\_S(#,#)
      - DEFAULT value of 0.0
- Define temperature
  1. Specification always available
  2. Input required when energy equations are solved
  3. Sets keyword BC\_T\_S(#,#)
  4. DEFAULT value of 293.15
- Select species and set mass fractions (table format)
  1. Specification always available
  2. Input required for species equations
  3. Drop down menu of solid species
  4. Sets keyword BC\_X\_S(#,#,#)
  5. DEFAULT - last defined species has mass fraction of 1.0
  6. Error check: mass fractions must sum to one

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(add) (remove) (copy)

Region	Boundary Type
Walls	No Slip Wall
Distributor	Mass Inflow

Fluid Sand Coal Scalar

Volume Fraction: 0.01

Y-Axial Velocity: 0.0 m/s

Tangential Velocity Components:

X-Axial Velocity: 0.0 m/s

Z-Axial Velocity: 0.0 m/s

Temperature: 293.15 K

Granular temperature: 0.0 TBD

Particles per parcel: 1.0

Species	Mass Fraction
Char	0.30
Ash	0.70

*Mockup of Task pane for specifying the Solids properties for MI, CG\_MI, and PI boundary condition regions.*

**Scalar (tab)** - Tab only available if scalar equations are solved

- Define initial scalar value
  - Sets keyword BC\_SCALAR(##)
  - DEFAULT value of 0.0

**Subtask Pane Tab for PRESSURE OUTFLOW type (PO) Boundary Condition Regions**

**Fluid (tab)**

- Define pressure
  - Specification always available
  - Input required
  - Sets keyword BC\_P\_G(#)
  - DEFAULT 101.325d3

*The remaining inputs are "optional." They do not have default values, because MFIX will calculate appropriate values if they are unspecified and 'backflow' occurs at the outlet.*

- Define volume fraction
  - Specification always available
  - Sets keyword BC\_EP\_G(#)
  - No DEFAULT value
  - Error Check: If any volume fraction for the BC region is specified, then all volume fractions for the BC region must be specified and must sum to one.
- Define temperature
  - Specification always available
  - NO DEFAULT value
  - Sets keyword BC\_T\_G(#)
- Select species and set mass fractions (table format)
  - Specification always available
  - NO DEFAULT value
  - Sets keyword BC\_X\_G(##)

4. Error check: if specified, mass fractions must sum to one\_

### **Solids-# (tab)**

*All inputs are optional. They do not have default values, because MFIX will calculate appropriate values if they are unspecified and 'backflow' occurs at the outlet.*

- Define volume fraction
  1. Specification always available
  2. Sets keyword BC\_EP\_S(,#, #)
  3. No DEFAULT value
  4. Error Check: If any volume fraction for the BC region is specified, then all volume fractions for the BC region must be specified and must sum to one.
- Define temperature
  1. Specification always available
  2. NO DEFAULT value
  3. Sets keyword BC\_T\_S(,#, #)
- Select species and set mass fractions (table format)
  1. Specification always available
  2. NO DEFAULT value
  3. Sets keyword BC\_X\_S(,#, #, #)
  4. Error check: if specified, mass fractions must sum to one\_

### **Scalar (tab)** - Tab only available if scalar equations are solved

*All inputs are optional. They do not have default values, because MFIX will calculate appropriate values if they are unspecified and 'backflow' occurs at the outlet.*

- Define scalar value
  1. Sets keyword BC\_SCALAR(,#, #)
  2. NO DEFAULT value

Geometry		(add) (remove) (copy)	
Mesh		Region	Boundary Type
Regions		Walls	No Slip Wall
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Fluid		P.Outflow	Pressure Outflow
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Fluid	Sand	Coal	Scalar
Pressure: <input type="text" value="101.325d3"/> Pa			
Optional Specifications:			
Volume Fraction: <input type="text"/>			
Temperature: <input type="text"/> K			
Species	Mass Fraction		
---	<input checked="" type="checkbox"/>	1.00	

Geometry		(add) (remove) (copy)	
Mesh		Region	Boundary Type
Regions		Walls	No Slip Wall
Model Setup		Distributor	Mass Inflow
Fluid		P.Outflow	Pressure Outflow
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Continuum Solids Model			
Initial Conditions			
<b>Boundary Conditions</b>			
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Internal Surfaces			
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Planes			
Volumes			
Run			

Fluid	Sand	Coal	Scalar
Optional Specifications:			
Volume Fraction: <input type="text"/>			
Temperature: <input type="text"/> K			
Species	Mass Fraction		
---	<input checked="" type="checkbox"/>	1.00	

**Subtask Pane Tab for MASS OUTFLOW type (MO) Boundary Condition Regions****Fluid (tab)**

- Define outflow properties: *Mass outflow specification changes based on the BC\_TYPE and Region orientation (e.g., XZ-Plane)*
  1. **For BC\_TYPE='MO' and XZ-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *Y-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_V\_G(#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_G(#)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_G(#)
        - DEFAULT value of 0.0
    - Define Tangential Velocities:
      - Define X-Axial Velocity
        - Sets keyword BC\_U\_G(#)
        - DEFAULT value of 0.0
      - Define Z-Axial Velocity
        - Sets keyword BC\_W\_G(#)
        - DEFAULT value of 0.0
  2. **For BC\_TYPE='MO' and YZ-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *X-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_U\_G(#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_G(#)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_G(#)
        - DEFAULT value of 0.0
    - Define Tangential Velocities:
      - Define Y-Axial Velocity
        - Sets keyword BC\_V\_G(#)
        - DEFAULT value of 0.0
      - Define Z-Axial Velocity
        - Sets keyword BC\_W\_G(#)
        - DEFAULT value of 0.0
  3. **For BC\_TYPE='MO' and XY-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *Z-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_W\_G(#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_G(#)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_G(#)

- DEFAULT value of 0.0
- Define Tangential Velocities:
  - Define X-Axial Velocity
    - Sets keyword BC\_U\_G(#)
    - DEFAULT value of 0.0
  - Define Y-Axial Velocity
    - Sets keyword BC\_V\_G(#)
    - DEFAULT value of 0.0
- 4. **For BC TYPE='CG MO'**
  - Specify all velocity components:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_G(#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_G(#)
      - DEFAULT value of 0.0
    - Define Z-Axial Velocity
      - Sets keyword BC\_W\_G(#)
      - DEFAULT value of 0.0
  - Define duration to average outflow rate.
    1. Specification always available
    2. Input required
    3. Sets keyword BC\_DT\_0(#)
    4. DEFAULT value of 0.1
    5. Error Check: Value should be positive (non-negative)
    6. *BC\_DT\_0 specification should persist across the gas and solids tabs. If the user sets it in the gas phase tab, but then changes it under a solids tab, a warning message indicating that this value is 'constant' across all phases should be given.*

*The remaining inputs are only required when either the mass or the volumetric flowrates are specified. They are not required if the velocities are given for the outlet.*

**Comment on MO Volume fractions:** The GUI should support two possible cases:

- 1) All volume fractions (gas and solids) for the mass outlet are defined and their sum totals one;
- 2) All volume fractions are undefined.

However, if the BC is defined with either a specified mass or volumetric flow rate, then all volume fractions must be defined.

*Side note: MFI-X allows some strange 'partially' defined volume fractions for mass outflows but these will not be supported within the GUI.*

- Define volume fraction
  1. Specification required for specified mass or volumetric flowrates.
  2. Input required
  3. Sets keyword BC\_EP\_G(#)
  4. DEFAULT value 1.0
  5. Error Check: If any volume fraction for the BC region is specified, then all volume fractions for the BC region must be specified and must sum to one.
- Define temperature
  1. Specification is required when solving the energy equations (ENERGY\_EQ == .TRUE.) or with mass or volumetric flowrates and (RO\_G0 == UNDEFINED)



2. DEFAULT value 293.15
3. Sets keyword BC\_T\_G(#)
- Select species and set mass fractions (table format)
  1. Specification is available with mass or volumetric flowrates when (R\_G0 == UNDEFINED)
  2. DEFAULT value 1.0 of last defined species
  3. Sets keyword BC\_X\_G(##)
  4. Error check: if specified, mass fractions must sum to one\_

### **Solids-# (tab)**

- Define outflow properties: *Mass outflow specification changes based on the BC\_TYPE and Region orientation (e.g., XZ-Plane)*
  1. **For BC TYPE='MO' and XZ-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *Y-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_V\_S(##)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_S(##)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_S(##)
        - DEFAULT value of 0.0
    - Define Tangential Velocities:
      - Define X-Axial Velocity
        - Sets keyword BC\_U\_S(##)
        - DEFAULT value of 0.0
      - Define Z-Axial Velocity
        - Sets keyword BC\_W\_S(##)
        - DEFAULT value of 0.0
  2. **For BC TYPE='MO' and YZ-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *X-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC\_U\_S(##)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m<sup>3</sup>/s)*
        - Sets keyword BC\_VOLFLOW\_S(##)
        - DEFAULT value of 0.0
      - *Mass Flowrate (kg/s)*
        - Sets keyword BC\_MASSFLOW\_S(##)
        - DEFAULT value of 0.0
    - Define Tangential Velocities:
      - Define Y-Axial Velocity
        - Sets keyword BC\_V\_S(##)
        - DEFAULT value of 0.0
      - Define Z-Axial Velocity
        - Sets keyword BC\_W\_S(##)
        - DEFAULT value of 0.0
  3. **For BC TYPE='MO' and XY-Plane region**
    - Select mass outflow specification type:
      - Available selections:
      - *Z-Axial Velocity (m/s)* [DEFAULT]

- Sets keyword BC\_W\_S(#,#)
    - DEFAULT value of 0.0
  - *Volumetric Flowrate (m<sup>3</sup>/s)*
    - Sets keyword BC\_VOLFLOW\_S(#,#)
    - DEFAULT value of 0.0
  - *Mass Flowrate (kg/s)*
    - Sets keyword BC\_MASSFLOW\_S(#,#)
    - DEFAULT value of 0.0
  - Define Tangential Velocities:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_S(#,#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_S(#,#)
      - DEFAULT value of 0.0
- 4. For BC TYPE='CG MO'**
- Specify all velocity components:
    - Define X-Axial Velocity
      - Sets keyword BC\_U\_S(#,#)
      - DEFAULT value of 0.0
    - Define Y-Axial Velocity
      - Sets keyword BC\_V\_S(#,#)
      - DEFAULT value of 0.0
    - Define Z-Axial Velocity
      - Sets keyword BC\_W\_S(#,#)
      - DEFAULT value of 0.0
  - Define duration to average outflow rate.
    1. Specification always available
    2. Input required
    3. Sets keyword BC\_DT\_0(#)
    4. DEFAULT value of 0.1
    5. Error Check: Value should be positive (non-negative)

*BC\_DT\_0 specification should persist across the gas and solids tabs. If the user sets it in the gas phase tab, but then changes it under a solids tab, a warning message indicating that this value is*

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(add) (remove) (copy)

Region	Boundary Type
Walls	No Slip Wall
Distributor	Mass Inflow
M.Outflow	Mass Outflow

Fluid Sand Coal

Y-Axial Velocity: 0.0 m/s

Tangential Velocity Components:

X-Axial Velocity: 0.0 m/s

Z-Axial Velocity: 0.0 m/s

Outflow Time Average: 1.0 s

Volume Fraction:

Pressure: Pa

Temperature: K

Species	Mass Fraction

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(add) (remove) (copy)

Region	Boundary Type
Walls	No Slip Wall
Distributor	Mass Inflow
M.Outflow	Mass Outflow

Fluid Sand **Coal**

Y-Axial Velocity: 0.0 m/s

Tangential Velocity Components:

X-Axial Velocity: 0.0 m/s

Z-Axial Velocity: 0.0 m/s

Outflow Time Average: 1.0 s

Volume Fraction:

Pressure: Pa

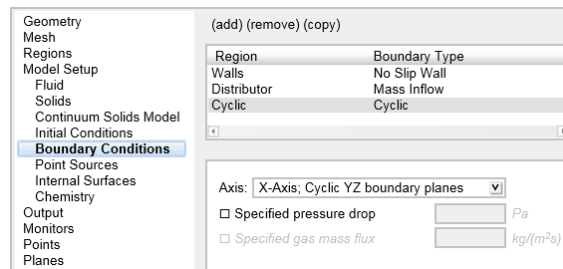
Temperature: K

Species	Mass Fraction

'constant' across all phases should be given.

### **Subtask Pane Tab for Cyclic type Boundary Conditions**

- Select cyclic axis
  1. Available selections
    - *X-Axis; Cyclic YZ boundary planes*
      - Sets keyword CYCLIC\_X to .TRUE.
    - *Y-Axis; Cyclic XZ boundary planes*
      - Sets keyword CYCLIC\_Y to .TRUE.
    - *Z-Axis; Cyclic XY boundary planes*
      - Sets keyword CYCLIC\_Z to .TRUE.
- Enable specified pressure drop
  1. DEFAULT value of .FALSE.
  2. Sets keyword based on axis:
    - *X-Axis; Cyclic YZ boundary planes*
      - Sets keyword CYCLIC\_X\_PD to .TRUE.
      - Required input for DELP\_X
        - DEFAULT value of 0.0
    - *Y-Axis; Cyclic XZ boundary planes*
      - Sets keyword CYCLIC\_Y\_PD to .TRUE.
      - Required input for DELP\_Y
        - DEFAULT value of 0.0
    - *Z-Axis; Cyclic XY boundary planes*
      - Sets keyword CYCLIC\_Z\_PD to .TRUE.
      - Required input for DELP\_Z
  3. Error check: Only one axis can have a specified pressure drop
  4. Error check: There should not be any BCs defined on walls that are cyclic. (I'm not sure if this check can be easily implemented.)
- Enable specified gas mass flux
  1. Requires specified pressure drop
  2. Sets keyword FLUX\_G
  3. DEFAULT value of 0.0
  4. Error check: Only one axis can have a specified mass flux. (This should not be an issue as it requires a specified pressure drop which can only be applied to one axis.)

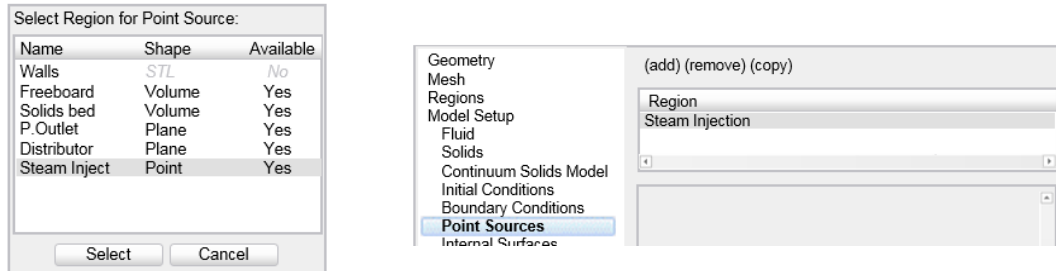


**Point Source Task Pane Window:** This section allows a user to define point sources for the described model. This section relies on regions named in the Regions section.

The top of the task pane is where users define/select PS regions

- Icons to add/remove/duplicate boundary conditions are given at the top

- Clicking the 'add' and 'duplicate' buttons triggers a popup window where the user must select a region to apply the point source.
  - Users cannot select inapplicable regions.
  - PS regions can be points, planes, or volumes (not STLs)
  - No region can define more than one point source.



Tabs group point source parameters for phases. Tabs are unavailable if no input is required from the user.

- Fluid tab - Unavailable if the fluid phase was disabled.
- Each solid phase will have its own tab. The tab name should be the name of the solid

### **Fluid (tab)**

- Define mass flowrate:
  - Select mass inflow specification type:
  - Sets keyword PS\_MASSFLOW\_G(#)
  - DEFAULT value of 0.0
- Define temperature
  - Specification only available when solving energy equations
  - DEFAULT value 293.15
  - Sets keyword PS\_T\_G(#)
- Select species and set mass fractions (table format)
  - Specification only available when solving species equations
  - DEFAULT value 1.0 of last defined species
  - Sets keyword PS\_X\_G(##)
  - Error check: if specified, mass fractions must sum to one
- Define X-axial velocity:
  - Specification always
  - No DEFAULT value (blank)
  - Sets keyword PS\_U\_G(#)
- Define Y-axial velocity:
  - Specification always
  - No DEFAULT value (blank)
  - Sets keyword PS\_V\_G(#)
- Define Z-axial velocity:
  - Specification always
  - No DEFAULT value (blank)
  - Sets keyword PS\_W\_G(#)

**Solids-# (tab)** - At this time, only TFM solids can be defined with point sources. At some point in the future, this could be extended to PIC solids, but never DEM.

- Define mass flowrate:
  4. Select mass inflow specification type:
  5. Sets keyword PS\_MASSFLOW\_S(##)
  6. DEFAULT value of 0.0
- Define temperature
  1. Specification only available when solving energy equations
  2. DEFAULT value 293.15
  3. Sets keyword PS\_T\_S(##)
- Select species and set mass fractions (table format)
  1. Specification only available when solving species equations
  2. DEFAULT value 1.0 of last defined species
  3. Sets keyword PS\_X\_S(##,##)
  4. Error check: if specified, mass fractions must sum to one
- Define X-axial velocity:
  1. Specification always
  2. No DEFAULT value (blank)
  3. Sets keyword PS\_U\_S(##)
- Define Y-axial velocity:
  1. Specification always
  2. No DEFAULT value (blank)
  3. Sets keyword PS\_V\_S(##)
- Define Z-axial velocity:
  1. Specification always
  2. No DEFAULT value (blank)
  3. Sets keyword PS\_W\_S(##)

**Internal Surfaces Task Pane Window:** This section allows a user to define internal surfaces for the described model. This section relies on regions named in the Regions section.

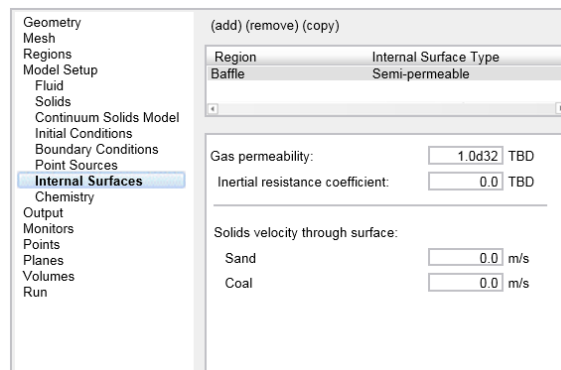
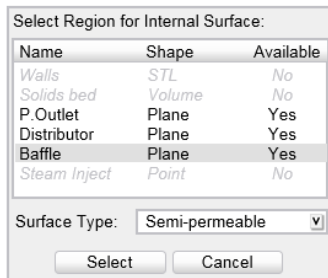
The top of the task pane is where users define/select IS regions

- Icons to add/remove/duplicate boundary conditions are given at the top
- Clicking the 'add' and 'duplicate' buttons triggers a popup window where the user must select a region to apply the internal surface.
  - Users cannot select inapplicable regions.
  - IS regions can be planes or volumes (not points or STLs)
  - No region can define more than one internal surface.
  -
- Select internal surface type
  - Selection is required
  - Available selections:
    - *Impermeable*
      - Selection only available for plane regions
      - set keyword IS\_TYPE(#) to 'IMPERMEABLE'
    - *X-Axis Impermeable*
      - Selection only available for volume regions
      - set keyword IS\_TYPE(#) to 'X\_IMPERMEABLE'
    - *Y-Axis Impermeable*
      - Selection only available for volume regions
      - set keyword IS\_TYPE(#) to 'Y\_IMPERMEABLE'
    - *Z-Axis Impermeable*
      - Selection only available for volume regions
      - set keyword IS\_TYPE(#) to 'Z\_IMPERMEABLE'
    - *Semi-permeable*

- Selection only available for plane regions
- set keyword IS\_TYPE(#) to 'SEMIPERMEABLE'
- *X-Axis semi-permeable*
  - Selection only available for volume regions
  - set keyword IS\_TYPE(#) to 'X\_SEMIPERMEABLE'
- *Y-Axis semi-permeable*
  - Selection only available for volume regions
  - set keyword IS\_TYPE(#) to 'Y\_SEMIPERMEABLE'
- *Z-Axis semi-permeable*
  - Selection only available for volume regions
  - set keyword IS\_TYPE(#) to 'Z\_SEMIPERMEABLE'
- DEFAULT - Impermeable

*Input is only needed for semi-permeable surfaces.*

- Gas permeability:
  1. Specification only available for semipermeable regions
  2. DEFAULT value 1.0d32
  3. Sets keyword IS\_PC(1)
- Internal resistance coefficient:
  1. Specification only available for semipermeable regions
  2. DEFAULT value 0.0
  3. Sets keyword IS\_PC(2)
- Solids velocity through surface:
  1. Specification only available for semipermeable regions
  2. DEFAULT value 0.0
  3. Sets keyword IS\_VEL\_s(1,PHASE)
  4. *There should be a line for each solids phase. Use the user provided solids name.*

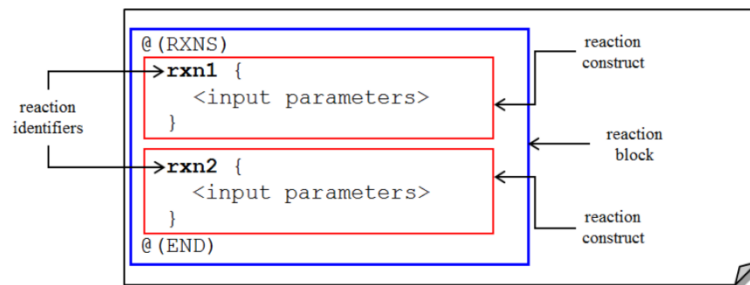


**Chemistry Task Pane Window:** This section allows a user to define chemical reaction input.

*Chemistry pane is disabled if any solids are specified as PIC.*

- Enable the stiff chemistry solver
  1. Selection always available
  2. Sets keyword STIFF\_CHEMISTRY to .TRUE.

Chemical reaction input is handled different than keyword pair inputs. All homogeneous gas phase chemical reactions and all heterogeneous gas-tfm solids reactions are specified between @ (RXNS) and @ (END) reaction block. All heterogeneous gas-dem and gas-pic reactions are specified between @ (DES\_RXNS) and @ (END) reaction block.



Users use the globally unique species aliases to specify the chemical reaction equation. Each reaction is specified with a unique reaction identifier.

- Specify the reaction identifier (Name)
  1. Specification always available
  2. DEFAULT value reactionN (for the Nth reaction)
  3. Reaction identifiers must be "Fortran compilable"
    - Alphanumeric combinations (no special characters excluding underscores)
    - Limited to 32 characters
    - First character must be a letter
    - No black spaces
- Specify chemical reaction reactants (table format)
  1. Use +/- buttons to add/remove reactants
  2. Column 1 - Select phase for reactant
    - Use drop down list of user defined phase names
    - Reactions are limited to homogeneous or two-phase heterogeneous reactions (e.g., species from three separate phases cannot be referenced by any single chemical reaction)
  3. Column 2 - Select reactant species
    - Use drop down list to show species in selected phase
    - A species can only appear once as a reactant in the same reaction
  4. Column 3 - Enter stoichiometric coefficient
    - Numerical value (integer or float)
    - Value must be non-negative
- Specify chemical reaction products (table format)
  1. Use +/- buttons to add/remove products
  2. Column 1 - Select phase for product
    - Use drop down list of user defined phase names
    - Reactions are limited to homogeneous or two-phase heterogeneous reactions (e.g., species from three separate phases cannot be referenced by any single chemical reaction)
  3. Column 2 - Select product species
    - Use drop down list to show species in selected phase
    - A species can only appear once as a product in the same reaction

4. Column 3 - Enter stoichiometric coefficient
  - Numerical value (integer or float)
  - Value must be non-negative
- Reactant/Product information is combined with stoichiometric coefficients to define the chemical reaction as a string.
  1. Sets reaction construct keyword CHEM\_EQ
  2. Example: CHEM\_EQ = "rcoeff1\*reactant1 + rcoeff2\*reactant2 --> pcoeff1\*product1"

**Error check:** Mass of the reactants equal mass of the products (within a tolerance, 1.0e-6).  
 $\text{abs}[(\text{rcoeff1} * \text{MW}(\text{reactant1}) + \text{rcoeff2} * \text{MW}(\text{reactant2}) - (\text{pcoeff1} * \text{product1}))] < 1.0\text{e-}6$

- Enable user-defined heat of reaction
  1. Selection always available
  2. DEFAULT disabled
- Specify heat of reaction
  1. Only available if user-defined heat of reaction is enabled
  2. DEFAULT value 0.0
  3. Sets reaction construct keyword DH
- Specify HoR fraction assigned to -phase-
  1. Only available if user-defined heat of reaction is enabled
  2. Homogeneous chemical reactions
    - Specification is not available
    - Set reaction construct keyword fracDH(#) to 1.0 where # is the phase index
  3. Heterogeneous chemical reactions
    - Entry for each phase referenced by the reaction
    - DEFAULT value 0.5 for both entires
    - Sets reaction construct keyword fracDH(#) for each referenced phase

Geometry  
Mesh  
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Continuum Solids Model  
Initial Conditions  
Boundary Conditions  
Point Sources  
Internal Surfaces  
**Chemistry**  
Output  
Monitors  
Run

(add) (remove) (copy)

Name	Stoichiometry
[Empty Row]	

☐ Enable stiff chemistry solver

Name: Char\_Combustion

Reactants: (add) (remove)

Phase	Species	Stoich. Coeff
Fluid	O2	1.00
Coal	Char	2.00

Products: (add) (remove)

Phase	Species	Stoich. Coeff
Fluid	CO	2.00

☐ Enable user-defined heat of reaction

Heat of reaction: [ ] J/mol

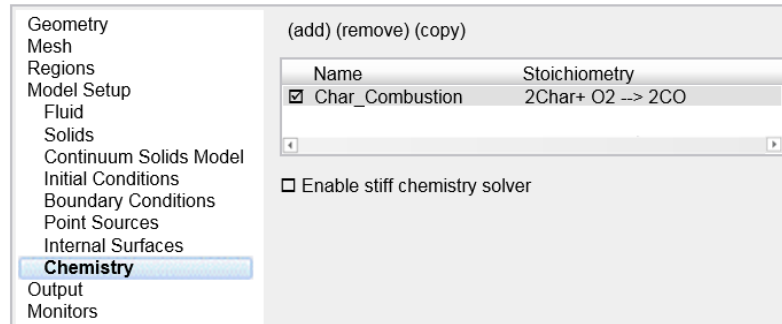
Fraction assigned to fluid: [ ]

Fraction assigned to coal: [ ]

Save Cancel



The user cannot 'save' the reaction if there are errors. After saving (adding?) the reaction, the reaction identifier (name) and chemical equation are shown in the summary box at the top. A chemical reaction is activated/deactivated by checking/unchecking the box. If the user 'deactivates' the chemical equation, the CHEM\_EQ reaction construct keyword should get set to "NONE."



### Numerics Task Pane Window:

*The numerics input is split into tabs to group similar inputs and reduce the amount of input needed on a single pane.*

#### Residuals (tab)

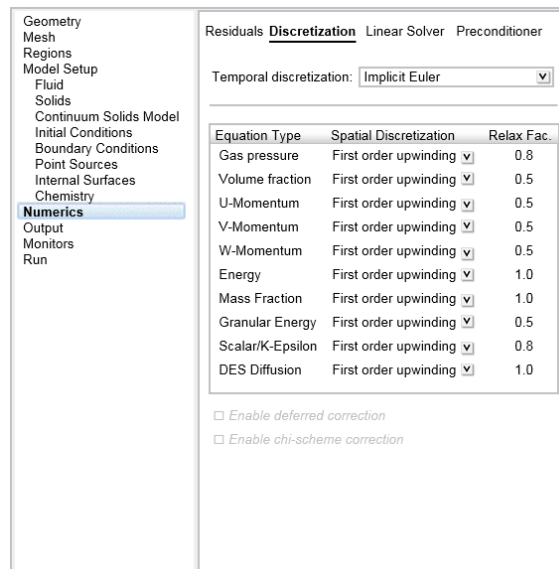
- Specify residual for continuity plus momentum equations
  1. Specification always available
  2. Sets keyword TOL\_RESID
  3. DEFAULT value of  $1.0e-3$
- Specify residual for energy equations
  1. Specification always available
  2. Sets keyword TOL\_RESID\_T
  3. DEFAULT value of  $1.0e-4$
- Specify residual for species equations
  1. Specification always available
  2. Sets keyword TOL\_RESID\_X
  3. DEFAULT value of  $1.0e-4$
- Specify residual for granular energy equations
  1. Specification always available
  2. Sets keyword TOL\_RESID\_TH
  3. DEFAULT value of  $1.0e-4$
- Specify residual for scalar/K-Epsilon
  1. Specification always available
  2. Sets keyword TOL\_RESID\_SCALAR
  3. DEFAULT value of  $1.0e-4$

Geometry Mesh Regions Model Setup Fluid Solids Continuum Solids Model Initial Conditions Boundary Conditions Point Sources Internal Surfaces Chemistry <b>Numerics</b> Output Monitors Run	<table border="1"> <thead> <tr> <th>Residuals</th> <th>Discretization</th> <th>Linear Solver</th> <th>Preconditioner</th> </tr> </thead> <tbody> <tr> <td colspan="4">Maximum residual at convergence</td> </tr> <tr> <td>Continuity + Momentum</td> <td></td> <td></td> <td>1.0e-3</td> </tr> <tr> <td>Energy</td> <td></td> <td></td> <td>1.0e-4</td> </tr> <tr> <td>Species</td> <td></td> <td></td> <td>1.0e-4</td> </tr> <tr> <td>Granular Energy</td> <td></td> <td></td> <td>1.0e-4</td> </tr> <tr> <td>Scalar/K-Epsilon</td> <td></td> <td></td> <td>1.0e-4</td> </tr> <tr> <td colspan="4">Minimum residual for divergence</td> </tr> <tr> <td></td> <td></td> <td></td> <td>1.0e+4</td> </tr> </tbody> </table>	Residuals	Discretization	Linear Solver	Preconditioner	Maximum residual at convergence				Continuity + Momentum			1.0e-3	Energy			1.0e-4	Species			1.0e-4	Granular Energy			1.0e-4	Scalar/K-Epsilon			1.0e-4	Minimum residual for divergence							1.0e+4
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Scalar/K-Epsilon			1.0e-4																																		
Minimum residual for divergence																																					
			1.0e+4																																		

### Discretization (tab)

- Select temporal discretization scheme
  1. Selection always available
  2. Available selections:
    - *Implicit Euler* [DEFAULT]
      - Sets keyword CN\_ON to .FALSE.
    - Crank-Nicholson
      - Sets keyword CN\_ON to .TRUE.
- Specify spatial discretization and under relation factors (table format)
  1. Specification always available
  2. Column 1: List of equations
  3. Column 2: Select discretization scheme for equation #
    - Available selections
      - *First-order upwind* [DEFAULT for all equations]
        - Sets keyword DISCRETIZE(#) to 0
      - *First-order upwind* (dwf)
        - Sets keyword DISCRETIZE(#) to 1
      - *Superbee*
        - Sets keyword DISCRETIZE(#) to 2
      - *SMART*
        - Sets keyword DISCRETIZE(#) to 3
      - *ULTRA-QUICK*
        - Sets keyword DISCRETIZE(#) to 4
      - *QUICKEST*
        - Sets keyword DISCRETIZE(#) to 5
      - *MUSCL*
        - Sets keyword DISCRETIZE(#) to 6
      - *van Leer*
        - Sets keyword DISCRETIZE(#) to 7
      - *minmod*
        - Sets keyword DISCRETIZE(#) to 8
      - Central
        - Sets keyword DISCRETIZE(#) to 9

4. Column 3: Specify under relation factors
  - Specification always available
  - Sets keyword UR\_FAC for each equation #
  - DEFAULTS are equation type specific
    - 1 - gas pressure: 0.8
    - 2 - volume fraction: 0.5
    - 3 - u-momentum: 0.5
    - 4 - v-momentum: 0.5
    - 5 - w-momentum: 0.5
    - 6 - energy: 1.0
    - 7 - species: 1.0
    - 8 - granular energy: 0.5
    - 9 - user-scalar/k-epsilon: 0.8
    - 10 - DES diffusion: 1.0
- Enable deferred correction
  1. Selection only available if minval(discretize) > 0
  2. Sets keyword DEF\_COR
  3. DEFAULT value .FALSE.
- Enable chi-scheme correction
  1. Selection only available if the species equation spatial discretization is SMART or MUSCL (DISCRETIZE(7) = 3 or 6)
  2. Sets keyword CHI\_SCHEME
  3. DEFAULT value .FALSE.



### Linear Solver (tab)

- Specify linear solver, number of iterations, and convergence tolerance (table format)
  1. Specification always available
  2. Column 1: List of equations
  3. Column 2: Select linear equation solver method for equation #
    - Available selections
      - BiCGSTAB [DEFAULT for all equations]
        - Sets keyword LEQ\_METHOD(#) to 2
      - GMRES

- Sets keyword LEQ\_METHOD(#) to 3
- 4. Column 3: Specify number of iterations
  - Specification always available
  - Sets keyword LEQ\_IT for each equation #
  - DEFAULTS are equation type specific
    - 1 - gas pressure: 20
    - 2 - volume fraction: 20
    - 3 - u-momentum: 5
    - 4 - v-momentum: 5
    - 5 - w-momentum: 5
    - 6 - energy: 15
    - 7 - species: 15
    - 8 - granular energy: 15
    - 9 - user-scalar/k-epsilon: 15
    - 10 - DES diffusion: 5
- 5. Column 4: Specify convergence tolerance
  - Specification always available
  - Sets keyword LEQ\_TOL
  - DEFAULT value of 1.0E-4 for all equations

Geometry	Residuals	Discretization	Linear Solver	Preconditioner
Mesh				
Regions				
Model Setup				
Fluid				
Solids				
Continuum Solids Model				
Initial Conditions				
Boundary Conditions				
Point Sources				
Internal Surfaces				
Chemistry				
<b>Numerics</b>				
Output				
Monitors				
Run				

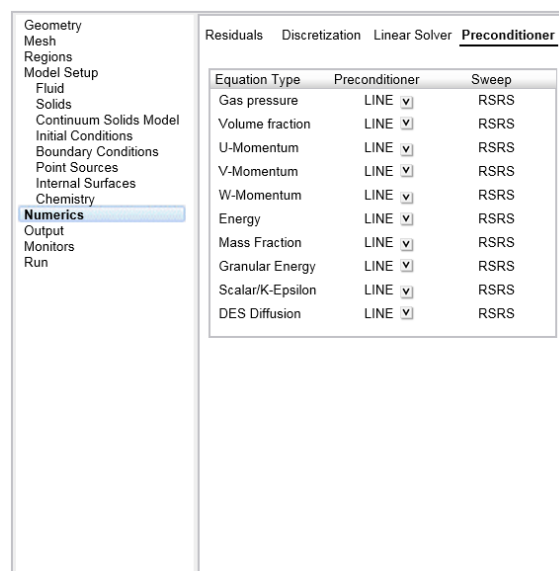
  

Equation Type	Solver	Iter.	Tol.
Gas pressure	BICGSTAB ▼	20	1.0e-4
Volume fraction	BICGSTAB ▼	20	1.0e-4
U-Momentum	BICGSTAB ▼	5	1.0e-4
V-Momentum	BICGSTAB ▼	5	1.0e-4
W-Momentum	BICGSTAB ▼	5	1.0e-4
Energy	BICGSTAB ▼	15	1.0e-4
Mass Fraction	BICGSTAB ▼	15	1.0e-4
Granular Energy	BICGSTAB ▼	15	1.0e-4
Scalar/K-Epsilon	BICGSTAB ▼	15	1.0e-4
DES Diffusion	BICGSTAB ▼	5	1.0e-4

### **Preconditioner (tab)**

- Specify linear solver, number of preconditioner and sweep direction (table format)
  1. Specification only available for equations using BiCGSTAB solver
  2. Column 1: List of equations
  3. Column 2: Preconditioner for equation #
    - Available selections
      - *None*
        - Sets keyword LEQ\_PC(#) to 'NONE'
      - *Line Relaxation* [DEFAULT for all equations]
        - Sets keyword LEQ\_PC(#) to 'LINE'
      - *Diagonal Scaling*
        - Sets keyword LEQ\_PC(#) to 'DIAG'

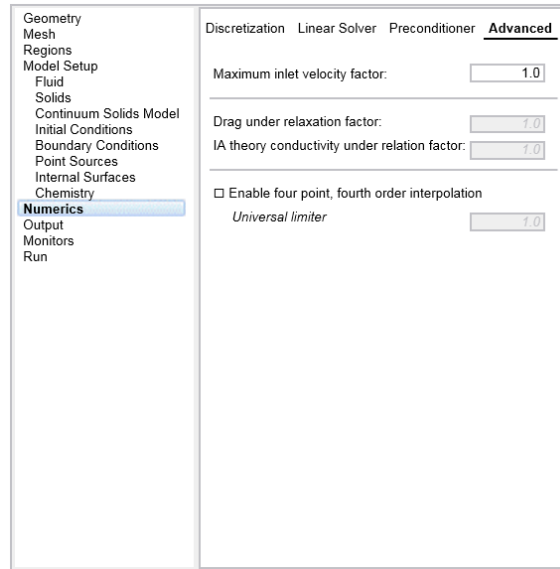
4. Column 3: Preconditioner sweep direction for equation #
- Selection only available for equations with LINE preconditioner
  - Available selections
    - *'Red-black sweep'* [DEFAULT for all equations]
      - Sets keyword LEQ\_PC(#) to 'RSRS'
    - *All sweep*
      - Sets keyword LEQ\_PC(#) to 'ASAS'
    - *I-sweep*
      - Sets keyword LEQ\_PC(#) to 'ISIS'
    - *J-sweep*
      - Sets keyword LEQ\_PC(#) to 'JSJS'
    - *K-sweep*
      - Sets keyword LEQ\_PC(#) to 'KSKS'



### Advanced (tab)

- Specify maximum inlet velocity factor
  1. Specification always available
  2. Sets keyword MAX\_INLET\_VEL\_FAC
  3. DEFAULT value of 1.0
  4. Error check: Value greater than or equal to 1.0
- Specify drag under relation factor
  1. Specification only available with MFX-TFM and MFX-Hybrid solvers
  2. Sets keyword UR\_F\_GS
  3. DEFAULT value of 1.0
  4. Error check: Value bounded between 0 and 1
- Specify IA theory conductivity under relation factor
  1. Specification only available with KT\_TYPE = 'IA\_NONEP'
  2. Sets keyword IA\_NONEP
  3. DEFAULT value of 1.0
  4. Error check: value bounded between 0 and 1
- Enable four point, fourth order interpolation
  1. Specification always available
  2. Sets keyword FPFOI

3. DEFAULT value of .FALSE.
- Specify the universal limiter
  1. Specification only available if four point, forth order interpolation is enabled
  2. Sets keyword C\_FAC
  3. DEFAULT value of 1.0
  4. Error check: value bounded between 0 and 1



### Output Task Pane Window:

- Specify Restart/Checkpoint Frequency
- Option to enable restart backups
  1. **Subtask Pane Tab for restart/checkpoint backups**
  2. Backup frequency (multiple of restart/checkpoint frequency)
  3. Number of backup copies to retain
- Option to enable SPx output format
  1. **Subtask Pane Tab for SPx output format**
  2. Write frequency of SPx files (table format)
- Option to enable VTK output format
  1. **Subtask Pane Tab for VTK output format**
  2. Write frequency of VTK output (table format)
- Option to enable NetCDF output
  1. **Subtask Pane Tab for NetCDF output format**
  2. Write frequency of NetCDF output (table format)
- Option to write particle data (*requires DEM or PIC solver*)
- Option to enable distributed I/O

### 3.1.3 Job submission/Interactive Control

This section describes the interface for running a job and how to interact with the running solver.

When the MFIX solver is launched the following actions are taken:

- 1) Initializes MPI for DMP enabled solvers.
- 2) Initializes OpenMP threads for SMP enabled solvers.



### 3.1.4 Workflow Mode

Workflow mode utilizes pyqtnode's graphical programming interface and provides a collection of MFIX specific blocks for creating, running, and post processing MFIX simulations. This is where design of experiments, uncertainty quantification, and optimization can be performed.

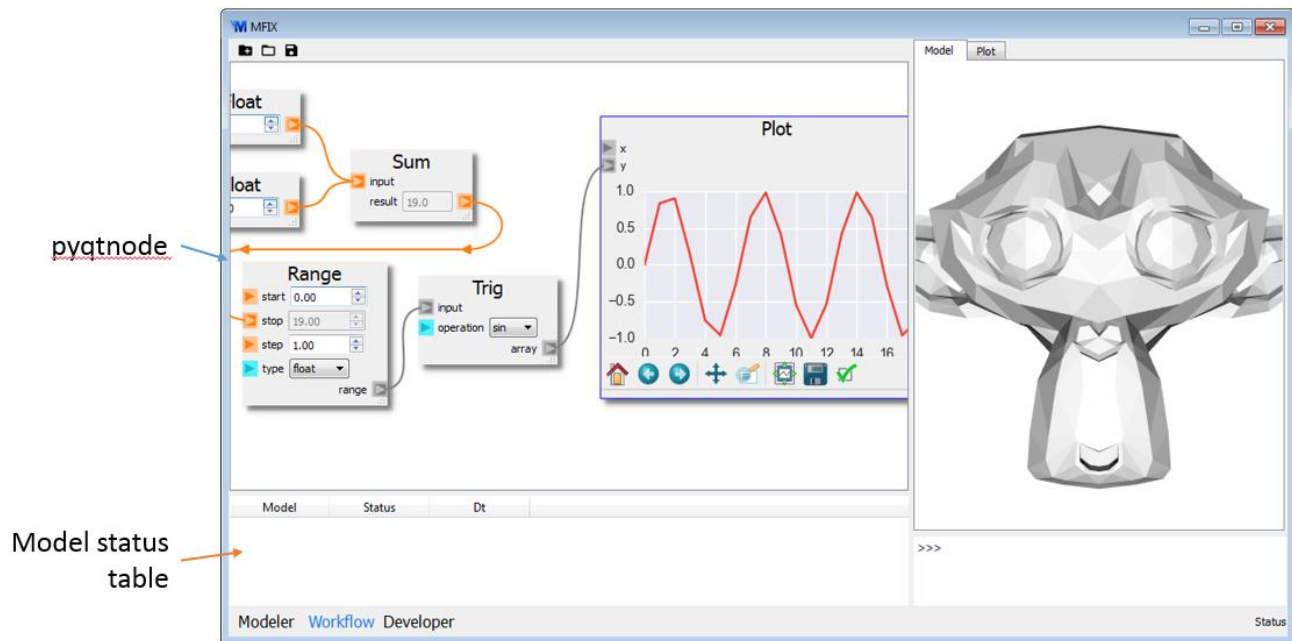
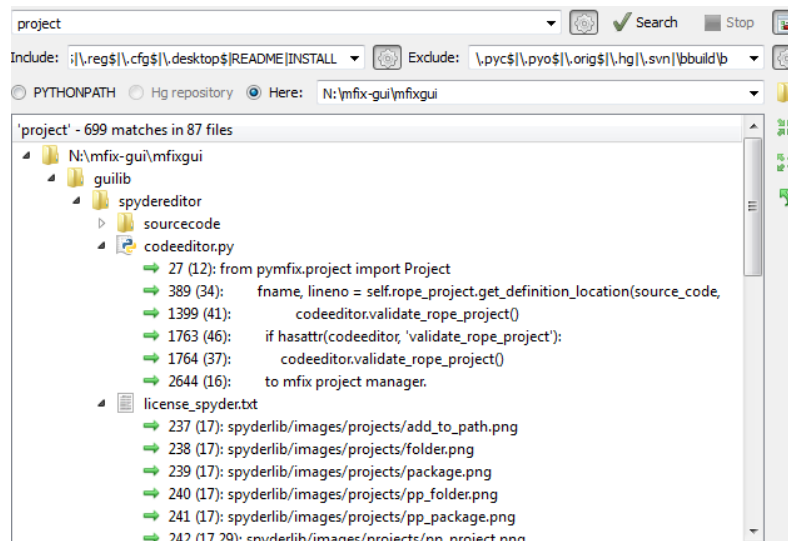


Figure 3: General layout of the “Workflow” mode.

### 3.1.5 Developer Mode

Developer mode allows users to edit user-defined functions (UDFs) and the MFIX-Solver source code. Developer mode also contains tools to help develop, maintain, and characterize performance of the MFIX-Solver source code.





The layout will consist of a tree on the left side showing the structure and files that compose the MFIX-Solver. There will also be a search bar that can either search the files names or search through the files and show where that specific search term exists in the files it has been found in.

*Screenshot of a neat tool in spyder for searching through code repositories with regular expressions. Indicates files and lines in files where the search has been found.*

A light-weight text editor should be included, providing FORTRAN syntax highlighting, tabbed completion, and inline error checking (Note: could use spyder's editor, however it seems to be sluggish and "heavy" sometimes, especially on the SBEUC).

## Hardware Interfaces

XBOX Kinetic control of the interface with hand motions ☺.

## Software Interfaces

- **Paraview:** The MFIX-UI should be able to open Paraview and ideally open a graphics file stack from the current simulation directory with a state file.
- **C3M:** Open C3M (available only on Windows)

## Communications Interfaces

- Interaction with a running simulation
  - The MFIX-UI will communicate with a running MFIX simulation over a user-specified port using a RESTful HTTP interface. The interface will be language neutral, using the JSON format for data exchange.
  - The status of a running MFIX simulation will be monitored by the MFIX-UI over HTTP.
- Interaction with the MFS Website
  - Read/display news
  - Import particle properties from the MFS particle database
  - Download updates?

- UDF repository?

## 4. System Features

### 4.1 Guided Simulation Setup

#### 4.1.1 Description and Priority

**High priority:** Specify an MFIX simulation through an intuitive user interface (UI). This feature should guide users in constructing a simulation by enabling/disabling features depending on selected options. For example, users should not be able to specify a kinetic theory model for non-Eulerian solids.

#### 4.1.2 Stimulus/Response Sequences

Users will be guided through a logic process for selecting model parameters.

#### 4.1.3 Functional Requirements

See section 3.

### 4.2 Internal Console

#### 4.2.1 Description and Priority

**High priority:** Create an interactive console that allows user manipulation of the model such as:

- Changing keywords
- Programmatically create BCs/ICs/PSs

As well as display relevant information including:

- Errors
- MFIX process connection info

#### 4.2.2 Stimulus/Response Sequences

When the user enters commands, process those commands and update the UI/model accordingly. Display relevant information from UI algorithms.

#### 4.2.3 Functional Requirements

- REQ-1: Display a console
- REQ-2: Allow user input
- REQ-3: Display information

### 4.3 3D Graphics - Visualization

#### 4.3.1 Description and Priority

**High priority:** Create a primitive 3D graphics environment to help visualize the simulation setup including:

- Displaying geometry

- Displaying the grid
- Displaying defined regions

#### 4.3.2 Stimulus/Response Sequences

As the user sets up the model, display relevant 3D objects to show geometry and regions.

#### 4.3.3 Functional Requirements

- REQ-4: Display the geometry (stl, primitives)
- REQ-5: Display Rectilinear grid overlaid with the geometry
- REQ-6: Display meshed geometry
- REQ-7: Display regions (point, plane, volume)

### 4.4 3D Graphics – Interaction

#### 4.4.1 Description and Priority

**Medium priority:** Provide user interactivity with the 3D environment for changing the size, rotation, and position of objects such as the geometry, grid, and regions.

#### 4.4.2 Stimulus/Response Sequences

The user will use mouse and keyboard inputs to change objects in the 3D space

#### 4.4.3 Functional Requirements

- REQ-1: Change the size, position, and rotation of geometry objects
- REQ-2: Move grid control points
- REQ-3: Change the size, position, and rotation of region objects
- REQ-4: Select individual cells/triangles

### 4.5 Geometric preprocessing

#### 4.5.1 Description and Priority

**High priority:** Create an mfix.dat file through the GUI.

#### 4.5.2 Stimulus/Response Sequences

As the user works through the interface, key, arguments, and values will be generated and stored in a data structure. When the user “saves” the project, the mfix.dat will be generated.

#### 4.5.3 Functional Requirements

- REQ-1: Collect and store correct keywords, arguments, and values  
Write the collected keywords

### 4.6 Installer

#### 4.6.1 Description and Priority

**High priority:** Create a self-contained installed program each targeted platform.

#### 4.6.2 Stimulus/Response Sequences

The user will download a single platform-specific installer file to install MFIX, the MFIX-UI, and all dependencies. PyInstaller will be used to bundle together the Python distribution and dependencies into a convenient installer.

#### 4.6.3 Functional Requirements

- REQ-1: Installation on Windows
- REQ-2: Installation on Linux (ubuntu, opensuse, fedora, ...)
- REQ-3: Installation on OSX

### 4.7 Creating mfix.dat

#### 4.7.1 Description and Priority

**High priority:** Create an mfix.dat file through the GUI.

#### 4.7.2 Stimulus/Response Sequences

As the user works through the interface, key, arguments, and values will be generated and stored in a data structure. When the user “saves” the project, the mfix.dat will be generated.

#### 4.7.3 Functional Requirements

- REQ-1: Collect and store correct keywords, arguments, and values
- REQ-2: Write the collected keywords, arguments, and values to a text file named mfix.dat

### 4.8 Building MFIX

#### 4.8.1 Description and Priority

**Medium priority:** Build MFIX

#### 4.8.2 Stimulus/Response Sequences

The user will select a button or menu item to build an MFIX executable from the MFIX source distributed with the MFIX UI.

#### 4.8.3 Functional Requirements

This capability is optional for the binary distribution of MFIX-UI, which will include a prebuilt MFIX executable, for the situation when the user does not have a compiler installed. Building MFIX through the GUI would be useful to rebuild with different build options: SMP, DMP, different Fortran compilers and MPI implementations.

- REQ-1: Build on Linux
- REQ-2: Build on OSX
- REQ-3: Build using Autotools

- REQ-4: Build using SMP
- REQ-5: Build using DMP

## 4.9 Running MFIX

### 4.9.1 Description and Priority

**High priority:** Start MFIX

### 4.9.2 Stimulus/Response Sequences

The user will select a menu item to launch MFIX locally, submit it to a batch queue, or connect to an already running MFIX simulation. The MFIX-UI will then display the progress of the job and various statistics.

### 4.9.3 Functional Requirements

- REQ-1: Remove existing run files
- REQ-2: Check to make sure a compiled MFIX source is available
- REQ-3: Copy required files
- REQ-4: Launch job locally
- REQ-5: Pause a running job
- REQ-6: Resume a job
- REQ-7: Update timestep
- REQ-8: Write restart (RES) files
- REQ-9: Terminate a job
- REQ-10: Reinitialize with an updated mfix.dat
- REQ-11: View a job's current simulation time, current timestep, residuals for current iteration of the current timestep, and estimated walltime to finish

## 4.10 Queue Support

### 4.10.1 Description and Priority

**High priority:** Allow for submitting/monitoring/canceling of jobs submitted to a queue manager.

### 4.10.2 Stimulus/Response Sequences

The user can select to submit a job to a specific queue.

### 4.10.3 Functional Requirements

- REQ-1: Flexible interface for users to specify queue parameters
- REQ-2: Submit job to a queue
- REQ-3: Monitor job status (waiting/running/canceled/ended)
- REQ-4: Remove job from queue
- REQ-5: Monitor queue availability and automatically move queued jobs to other queues

## 4.11 External Programs

### 4.11.1 Description and Priority

**Medium Priority:** After running MFIX, provide a button to open simulation results in Paraview.

#### 4.11.2 Stimulus/Response Sequences

The user will select a menu item to launch MFIX simulation results in Paraview. Ideally, this will include opening the graphics stack and applying a state file.

#### 4.11.3 Functional Requirements

- REQ-1: Launch Paraview by pressing a button in the UI
- REQ-2: Open the current simulation's graphics stack in Paraview
- REQ-3: Set a state file to setup the visualization in Paraview

### 4.12 Plugins

#### 4.12.1 Description and Priority

**Medium Priority:** Provide a structure for user supplied plugins

#### 4.12.2 Stimulus/Response Sequences

Users will be able to create plugins for the UI to handle:

- queue submissions
- widgets
- Post processing

#### 4.12.3 Functional Requirements

- REQ-1: Automatically look for plugins
- REQ-2: expose the plugin in the UI

### 4.13 Pyqtnode Interaction

#### 4.13.1 Description and Priority

**High Priority:** import the pyqtnode library and display under the "workflow" mode.

#### 4.13.2 Stimulus/Response Sequences

The user will select the "workflow" mode where the UI will change to show the pyqtnode interface. Run and autorun buttons will be exposed.

#### 4.13.3 Functional Requirements

- REQ-1: Import pyqtnode and imbed in the UI
- REQ-2: expose hooks for pyqtnode to run MFIX simulations

## 4.14 Species Database

### 4.14.1 Description and Priority

**High Priority:** Include a large collection of thermodynamic species data that a user can “import” into the model.

Database links: <http://webbook.nist.gov/chemistry/>,  
<http://www.grc.nasa.gov/WWW/CEAWeb/ceaThermoBuild.htm>

### 4.14.2 Stimulus/Response Sequences

Where needed, a user can search and import gas, liquid, and solids species from a database.

### 4.14.3 Functional Requirements

- REQ-1: Include a thermodynamic data base with the UI  
REQ-2: Import species data from that data base

## 5. Other Nonfunctional Requirements

### Performance Requirements

The UI should not “hang” during operations that require significant amounts of time (> 1s) to complete. Example actions that could take significant time include:

- Reading stl files
- Sending interaction requests to a running MFIX simulation
- Receiving data from a running MFIX simulation
- Compiling MFIX

### Safety Requirements

If the UI removes any files from the user’s system, a prompt must be displayed asking the user to continue.

### Security Requirements

User names and passwords for access to the MFS (mfix.netl.doe.gov) website should be stored (encrypted) securely.

### Software Quality Attributes

The software must be written in a modular and flexible fashion, allowing for maintainability, reusability, and robustness. Documentation, “docstrings”, should be included with function, class, and method definitions. All functions, classes, and methods should be unit-testable. Unit tests should be written for every function, class, and method as the functions, classes, and methods are developed, **NOT AS AN AFTERTHOUGHT**.

## Code Style Guide

All Python code should follow the standard Python style guide. If your editor supports it, please enable pylint checking.

## Business Rules

*<List any operating principles about the product, such as which individuals or roles can perform which functions under specific circumstances. These are not functional requirements in themselves, but they may imply certain functional requirements to enforce the rules.>*

## 6. Other Requirements

*<Define any other requirements not covered elsewhere in the SRS. This might include database requirements, internationalization requirements, legal requirements, reuse objectives for the project, and so on. Add any new sections that are pertinent to the project.>*

## Appendix A: Glossary

*<Define all the terms necessary to properly interpret the SRS, including acronyms and abbreviations. You may wish to build a separate glossary that spans multiple projects or the entire organization, and just include terms specific to a single project in each SRS.>*

## Appendix B: Analysis Models

*<Optionally, include any pertinent analysis models, such as data flow diagrams, class diagrams, state-transition diagrams, or entity-relationship diagrams.>*

## Appendix C: To Be Determined List

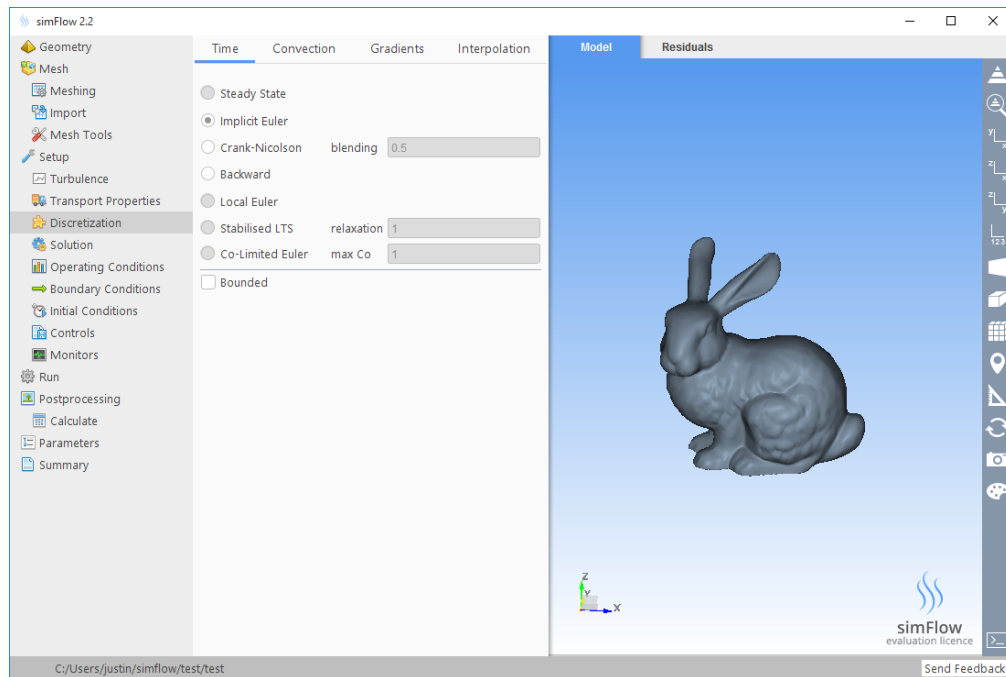
*<Collect a numbered list of the TBD (to be determined) references that remain in the SRS so they can be tracked to closure.>*

## Appendix D: UI Resources

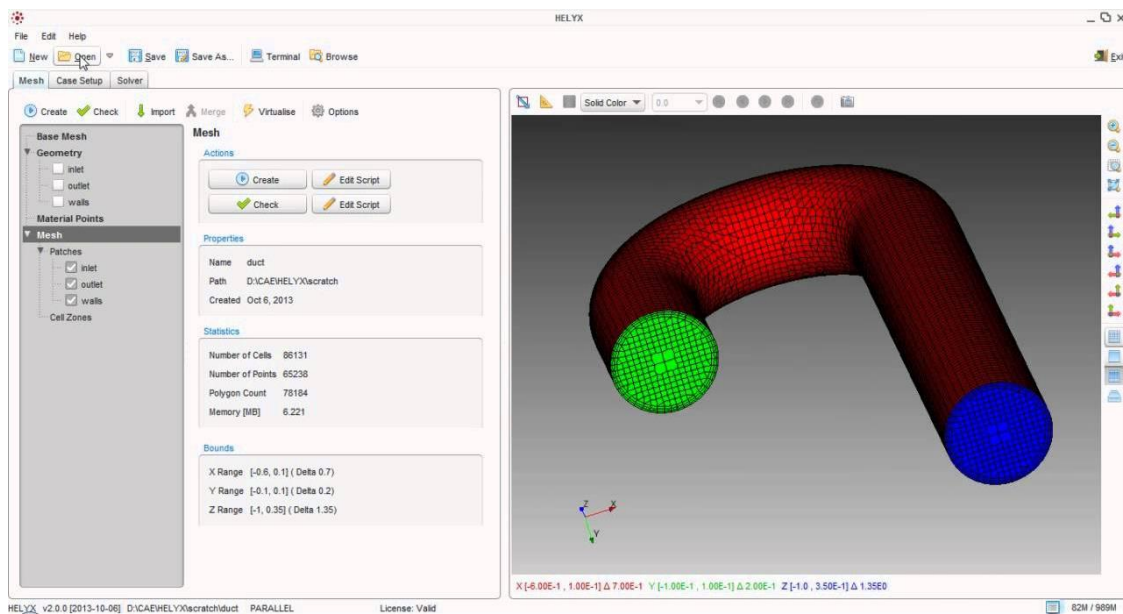
### Other CFD UI's



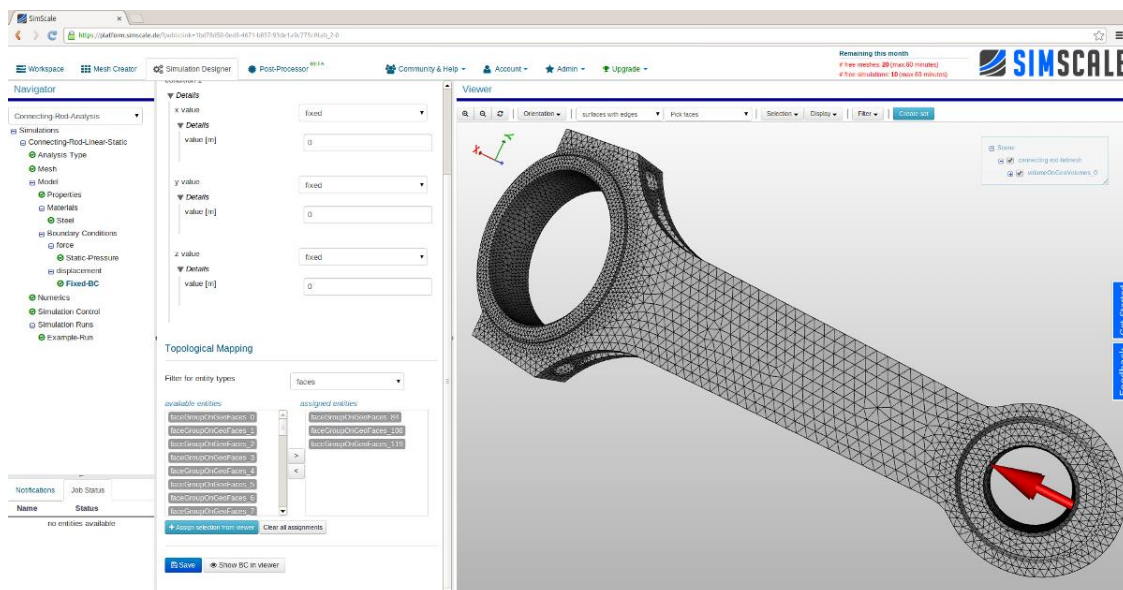
## SimFlow



## HELYX-OS



## SimScale



# DICEhub

