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.

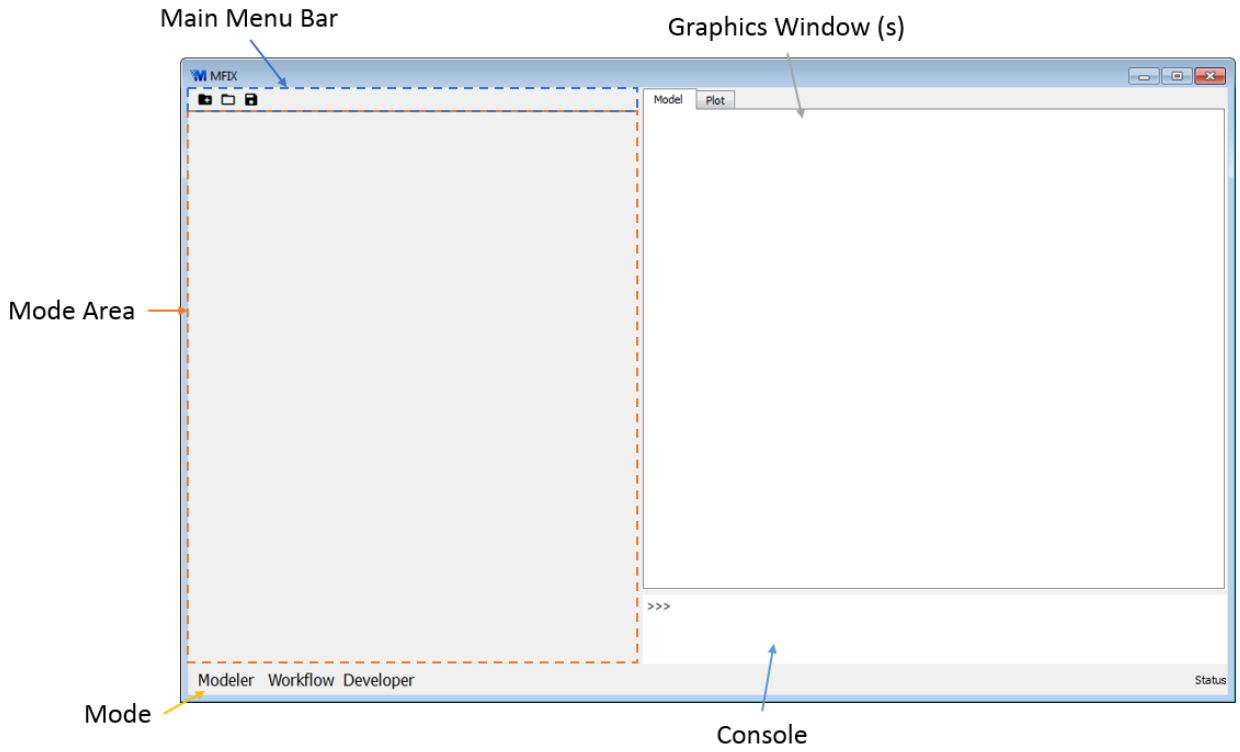
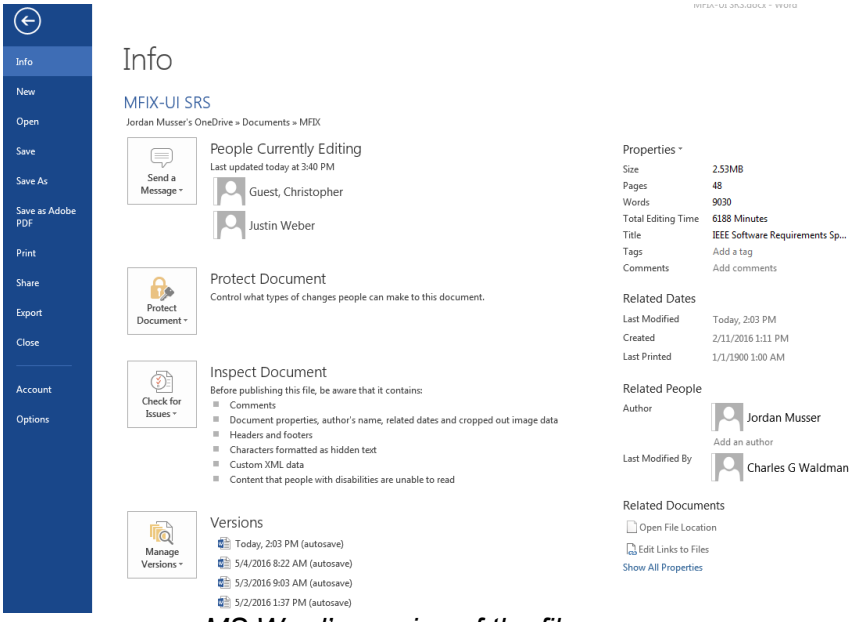


Figure 1: Basic layout of UI

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.

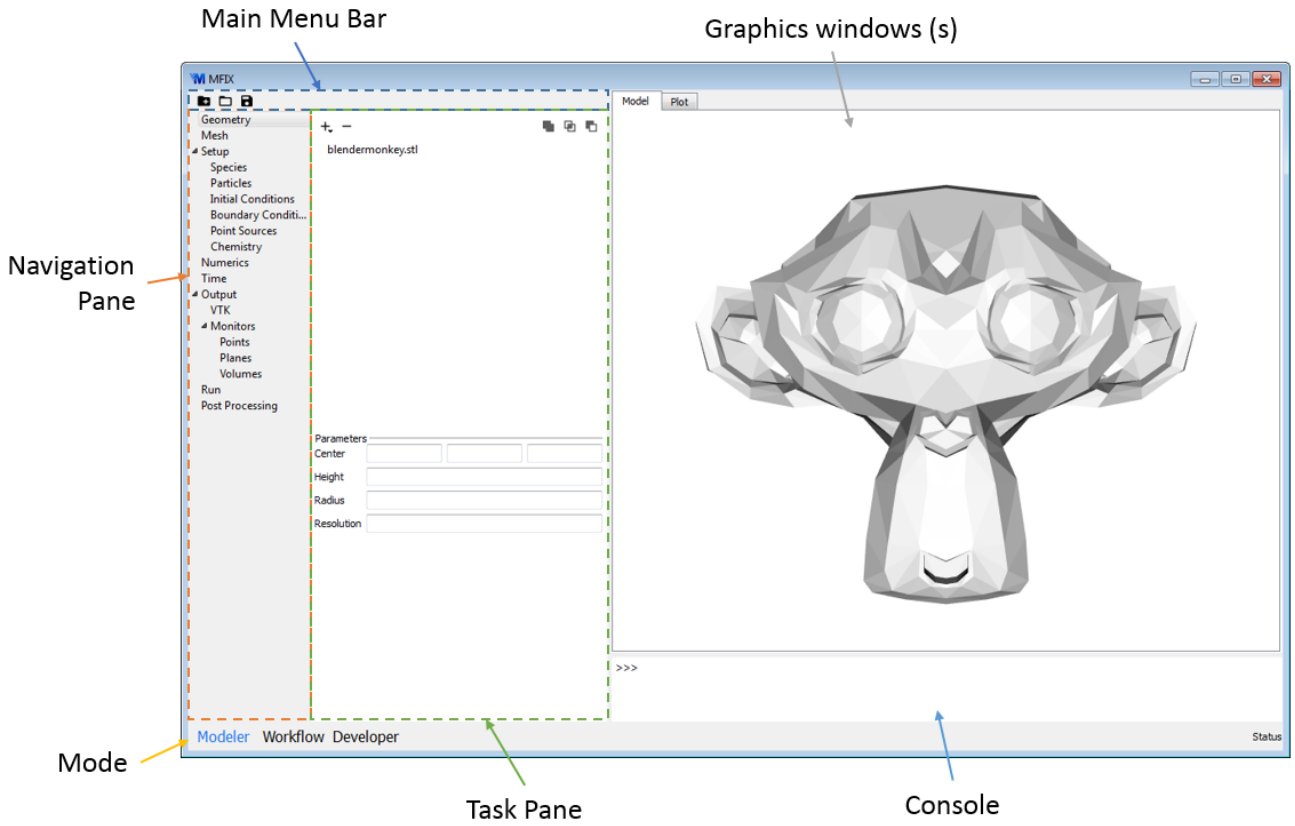


Figure 2: General layout of the Modeler mode

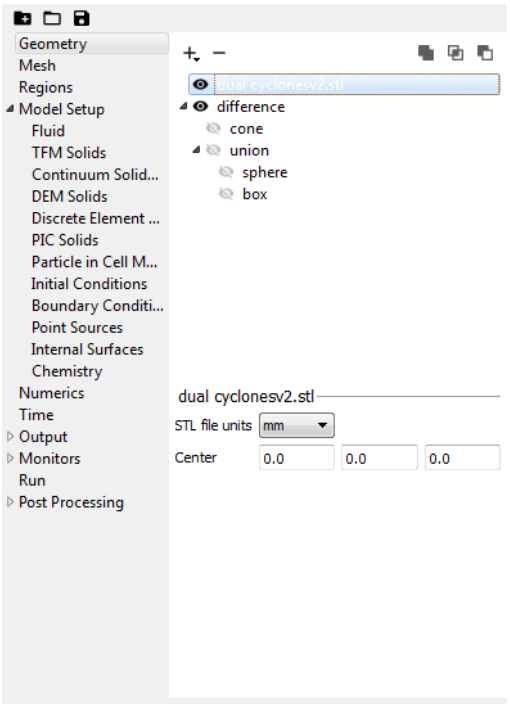
Navigation Pane:

- Geometry
- Mesh
- Regions
- Model Setup
  - Fluid (*available unless disabled in solver task pane*)
  - 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*)
  - Initial Conditions
  - Boundary Conditions
  - Point Sources
  - Internal Surfaces
  - Chemistry
- Numerics
- Output
- Monitors
  - Points
  - Planes
  - Volumes
- Run
- Post Processing

- Export
- Plugins

Geometry Task Pane Window: *Load/create geometry*

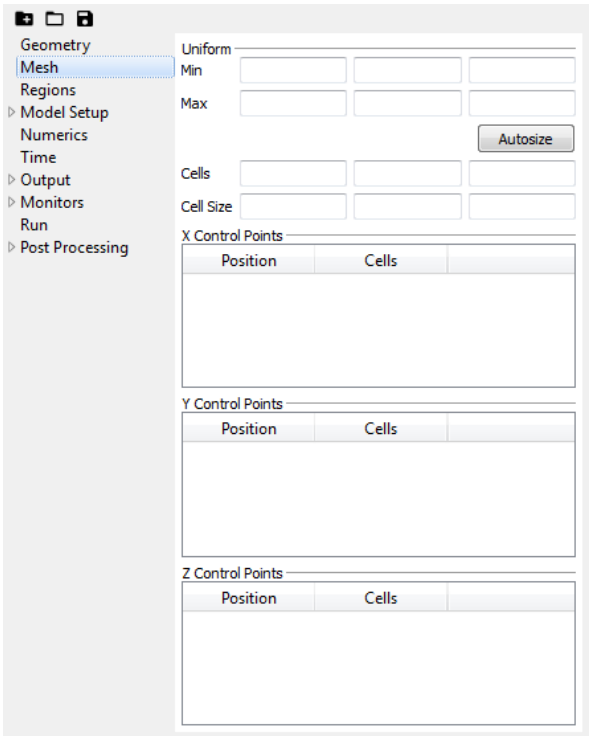
- Specify stl file(s)
- Specify primitive(s) (box, sphere, cylinder, cone)
- Apply filters
  - vtkCleanPolyData, vtkFillHolesFilter, vtkTriangleFilter, vtkDecimate, vtkDecimatePro, vtkQuadricDecimation, vtkQuadricClustering
- Perform boolean operations (union, difference, intersect)
- Edit geometry parameters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



Mockup of geometry task plane.

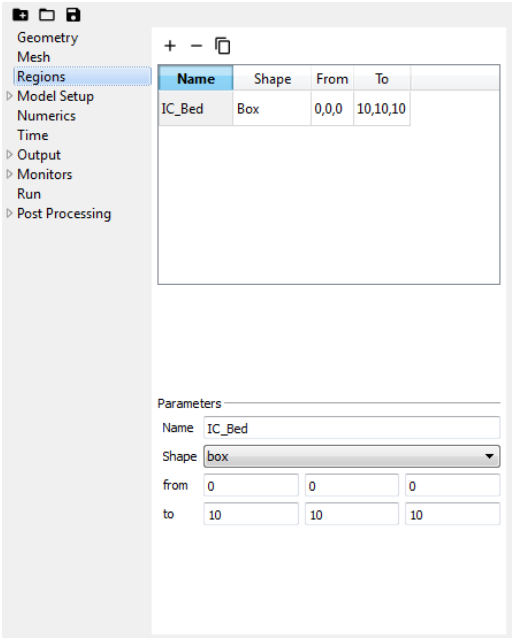
Mesh Task Pane Window: *Specify/Generate 3D Cartesian mesh*

- 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



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)

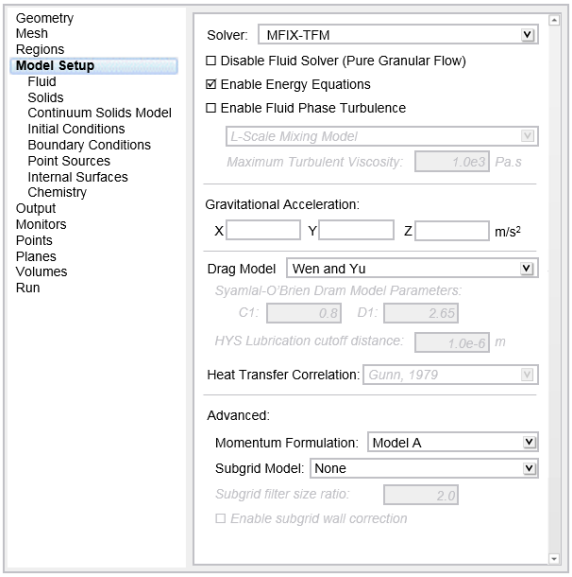


Model Setup Task Pane Window: *Select MFIX solver and other conservation equations*

- Select MFIX Solver:
  - 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
    - *MFIX-TFM*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Continuum Solids Model' task pane menu
    - *MFIX-DEM*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Discrete Element Model' task pane menu
    - *MFIX-PIC*
      - Selection *enables* 'Solids' task pane menu
      - Selection *enables* 'Particle-in-Cell' task pane menu
    - *MFIX-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
  - Disables the 'Fluid' task pane menu
  - Sets keyword RO_G0 to 0.0
- Option to enable thermal energy equations
  - This keyword should always be specified in the input deck
  - Sets keyword ENERGY_EQ
  - DEFAULT value of .FALSE.
- Option to enable turbulence
  - Selection available if fluid phase is enabled

    - 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)
    - Selection available if TURBULENCE_MODEL =/ 'NONE'
    - Sets keyword MU_GMAX
    - DEFAULT value of 1.0e3 (Pa.s)
- Specify Gravitational acceleration
    - Specification always available
    - Sets keywords GRAVITY_X, GRAVITY_Y, GRAVITY_Z
    - DEFAULT values
        - Leave blank when converting dat files to mfx
        - New cases take the values from the mfix.dat.template
    - If keyword GRAVITY is specified
        - GRAVITY_Y = -GRAVITY
        - GRAVITY_X = GRAVITY_Z = 0.0
- Specify drag model
    - Selection requires TFM, DEM, or PIC solver
    - Sets keyword DRAG_TYPE
    - 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 MFIX is limited in heat HTCs.*
- Specify momentum equation formulation; *Select Model A, Model B; Jackson, Ishii*
- Select sub-grid model:
    - Selection requirements:
        - Only available with MFIX-TFM solver

        - DRAG_TYPE="WEN_YU"
        - KT_TYPE="ALGEBRAIC"
        - TURBULENCE_MODEL /= K_EPSILON
        - BLENDING_STRESS = NONE
        - FRICTION_MODEL /= SRIVASTAVA
        - (There are more restrictions…)
    - Sets keyword SUBGRID_TYPE
    - Available selections
        - *NONE* (DEFAULT)
        - *IGCI*
        - *MILIOLI*
- Specify sub-grid model filter size ratio:
    - Specification requires SUBGRID_TYPE =/ NONE
    - Sets keyword FILTER_SIZE_RATIO
    - DEFAULT value of 2.0
- Enable sub-grid wall correction model:
    - Specification requires SUBGRID_TYPE =/ NONE
    - Sets keyword SUBGRID_WALL
    - DEFAULT value of FALSE



Mockup of Task pane for defining the Model Setup.

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

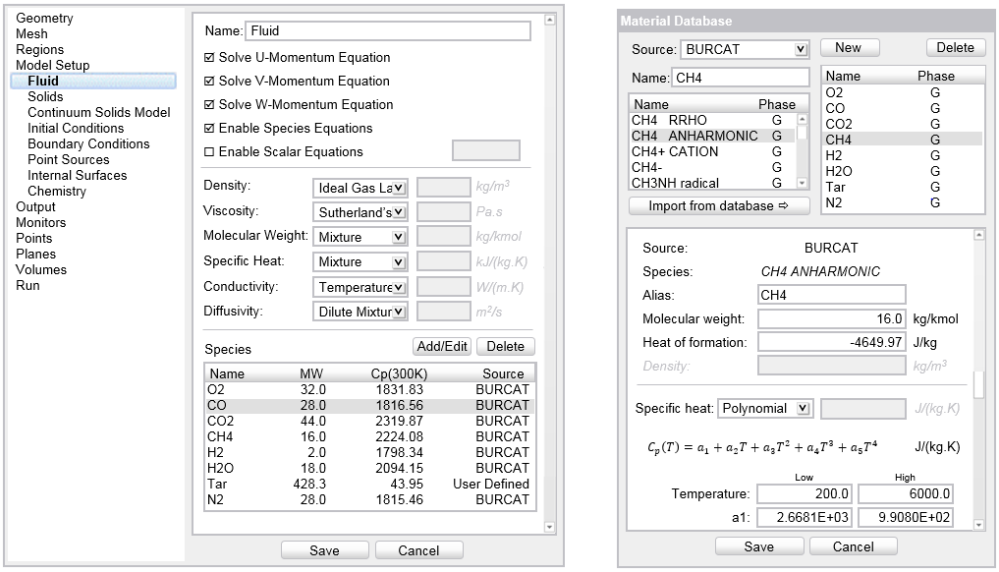
- Option to rename the phase (e.g, air, gas)
- Option to disable Momentum Equations (*enabled by default*)
    - Sets keyword: MOMENTUM_X/Y/Z_EQ(0)
- Option to enable Species Equations
    - Sets keyword: SPECIES_EQ(0)
    - Species Equations disabled [DEFAULT]
- Option to enable scalar equations
    - Define the number of scalar equations
    - Value sums into keyword NSCALAR
    - Sets keyword PHASE4SCALAR(*)=0 for total listed scalars

- Select Density Model:
  - Selection always available
  - 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
      - MFIX runtime check verifies UDF was provided
- Select Viscosity Model:
  - Selection always available
  - 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
      - MFIX runtime check verifies UDF was provided
- Select Molecular Weight Model:
  - Selection always available
  - 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:
  - Selection available only when solving thermal energy equations
  - 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
      - MFIX runtime check verifies UDF was provided
- Select Thermal Conductivity Model:
  - Selection only available when solving thermal energy equations

    - 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:
    - Selection only available when solving species equations
    - 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:
    - 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
    - Specification panel operates as a popup window triggered by an Add/Edit button
    - Summary window provides a list of the species and an overview of some properties
- Specify reference pressure
    - Specification requires fluid phase (RO_G0 /= 0.0)
    - Sets keyword P_REF
    - DEFAULT value of 0.0 (set in mfix.dat.template)
- Specify pressure scale factor
    - Specification requires fluid phase (RO_G0 /= 0.0)
    - Sets keyword P_SCALE
    - DEFAULT value 1.0 (set in mfix.dat.template)

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’



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:

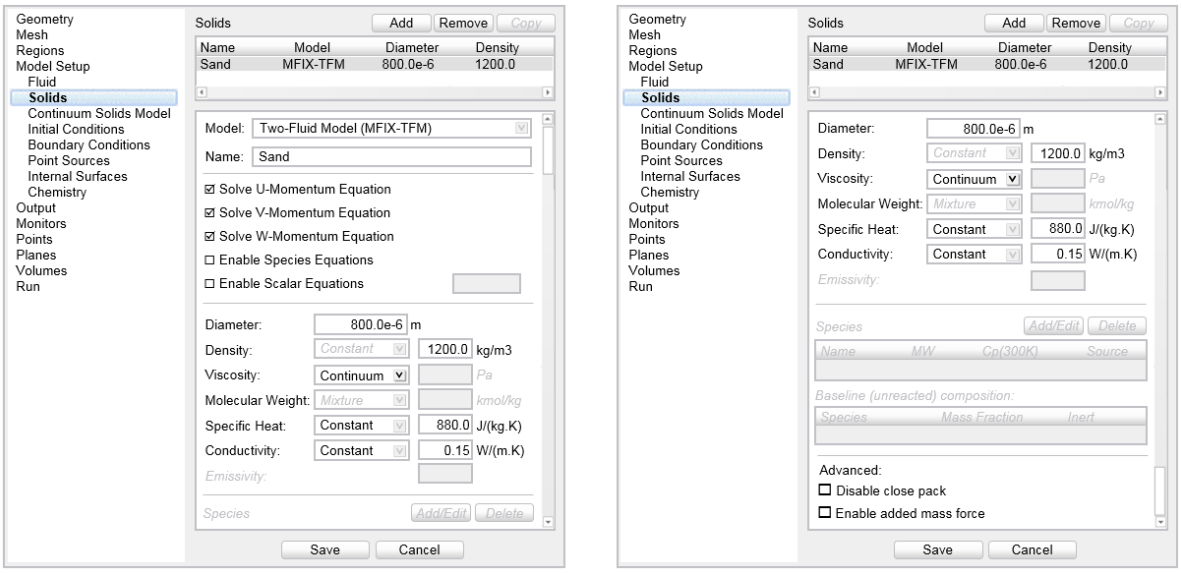
- Select Solids model
  - Sets keyword SOLIDS_MODEL(#)
  - Selection locked to Two-Fluid Model (MFIX-TFM) for MFIX-TFM solver
  - Selection locked to Discrete Element Model (MFIX-DEM) for MFIX-DEM solver
  - Selection locked to Multiphase Particle-in-Cell (MFIX-PIC) for MFIX-PIC solver
  - Selections available for MFIX-Hybrid solver
    - Two-Fluid Model (MFIX-TFM)
    - Discrete Element Model (MFIX-DEM)
- Option to give the phase a referenceable name (e.g., coal, sand)
  - Default to Solid-#
- Option to solve Momentum Equations
  - Selection only available for MFIX-TFM solids model
  - Sets keyword: MOMENTUM_X/Y/Z_EQ(#)
  - Moment equations enabled [DEFAULT]
- Option to enable Species Equations
  - Sets keyword: SPECIES_EQ(#)
  - Species Equations disabled [DEFAULT]
- Option to enable scalar equations

        - Selection only available for MFIX-TFM solids model
        - Define the number of scalar equations
        - Value sums into keyword NSCALAR
        - Sets keyword PHASE4SCALAR(*)=# for total listed scalars
- Specify Diameter (*required*)
    - Sets keyword: D_p0(#)
- Select Solids Density model
    - Selection requires species equations
    - 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, RO_XS0(#,#)
            - Requires base composition be specified, X_S0(#,#)
            - Requires an inert species be identified, INERT_SPECIES(#)
- Select Solids Viscosity Model:
    - Selection only available for MFIX-TFM solids model
    - 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
            - MFIX runtime check verifies UDF was provided
- Select Molecular Weight Model:
    - Selection available. Always locked to *Mixture*.
    - Available selections:
        - *Mixture* [DEFAULT]
            - Selection always available
            - Requires molecular weights for all species components
- Select Specific Heat Model:
    - Selection available only when solving thermal energy equations
    - 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(#)

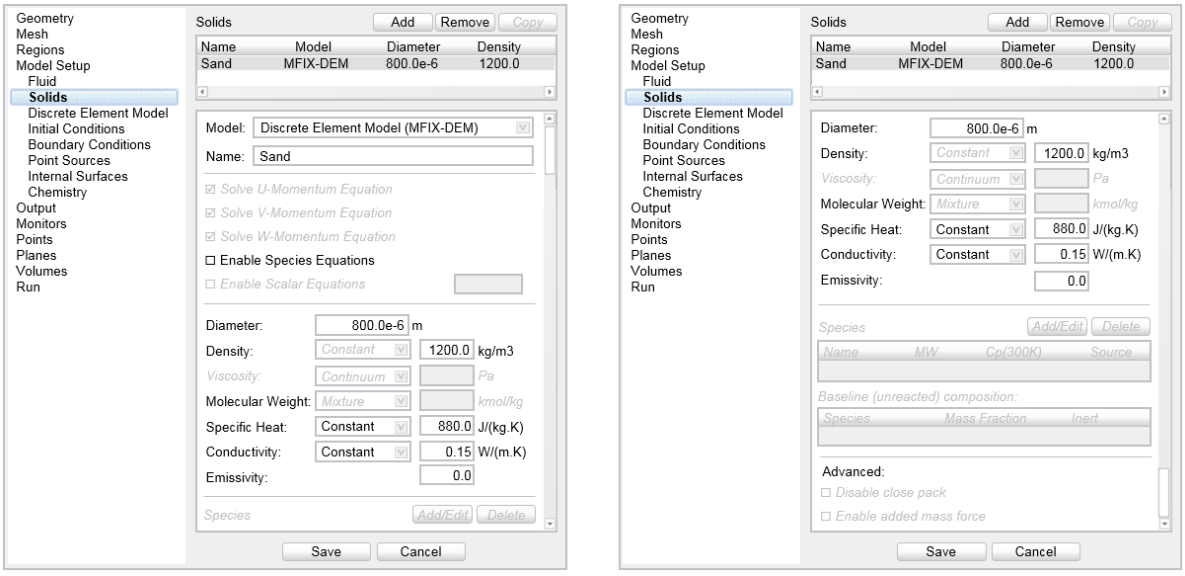
        - MFIX runtime check verifies UDF was provided
- Select Thermal Conductivity Model:
    - Selection only available for MFIX-TFM solids model
    - Selection only available when solving thermal energy equations
    - Available selections:
        - *Constant* [Locked DEFAULT for MFIX-DEM, MFIX-PIC]
            - 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(#)
            - MFIX runtime check verifies UDF was provided
- Specify solids phase emissivity
    - Selection only available for MFIX-DEM solids model
    - Specification only available when solving energy equations
    - Sets keyword DES_EM(#)
- Solids phase species selection:
    - Total number of species for each phase must be specified, NMAX_S(#)
    - Species data required under any of the following conditions:
        - Solving species equations
        - Energy equations are solved with mixture specific heat model
    - Specification panel operates as a popup window triggered by an Add/Edit button
    - Summary window provides a list of the species and an overview of some properties
    - Variable solids density requires users to specify the material density for each species
        - Sets keyword RO_XS0(#,#)
        - Value must be positive, non-zero
- Baseline (unreacted) composition selection:
    - Available only for variable solids density model
    - Select the solids phase species that comprise the initial particle composition
    - Specify initial mass fractions of the unreacted species, X_s0(#,#)
    - Mark one species as an inert material, INERT_SPECIES(#)

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

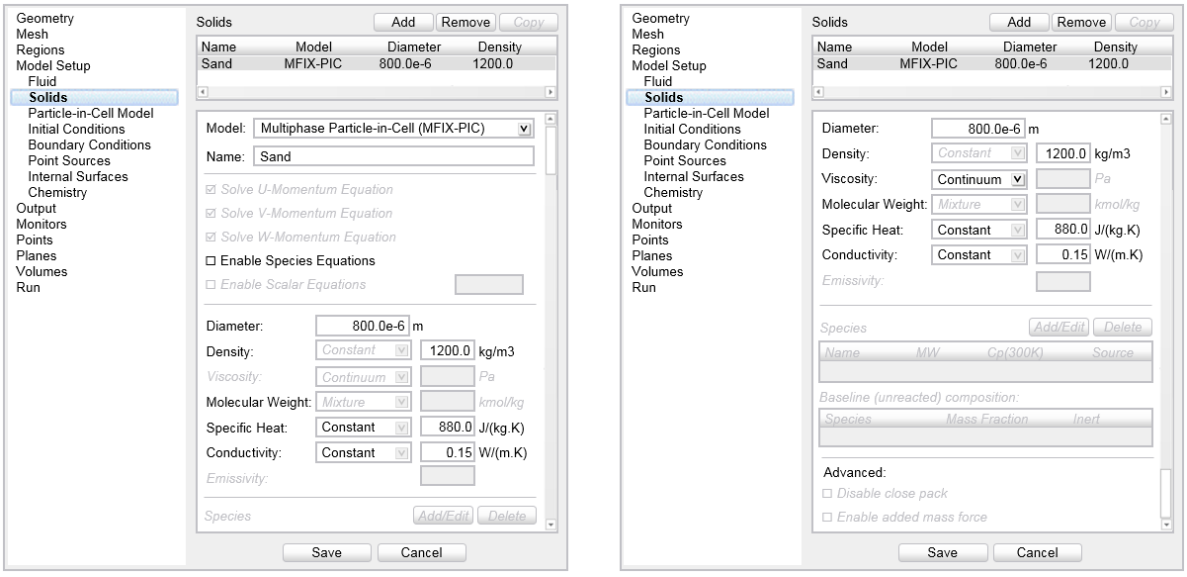
- Option to disable close packing
    - Selection only available for MFIX-TFM solids model
    - Sets keyword CLOSE_PACKED(#) = .FALSE.
    - Disabling close pack triggers a popup warning message.
- Option to include added mass force
    - Selection only available for MFIX-TFM solids model
    - Sets keyword ADDED_MASS and M_AM=#
    - Note: Only one phase can have added mass force



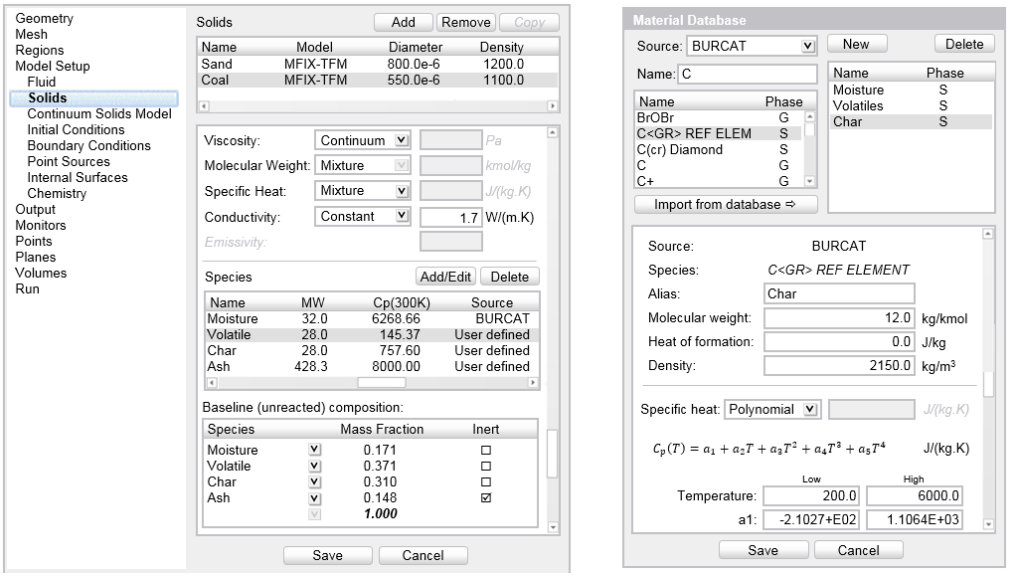
Mockup of Task pane for adding non-reacting TFM solids. Clicking the 'Save' button creates the solids phase whereas the 'Cancel' button resets all data fields to the default. In this mockup, solids are listed in a table as they are created. ***Left:*** *Top of the task pane.* ***Right:*** *Bottom of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



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*



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*)

- Sets keyword EP_STAR
- Select Viscous Stress Model (KTGS):
  - Selection is unavailable for constant solids viscosity (MU_S0 defined)
  - 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
  - Selection is unavailable for constant solids viscosity (MU_S0 defined)
  - 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
  - Only available with FRICTION_MODEL=SRIVASTAVA
  - Default value of 0.5

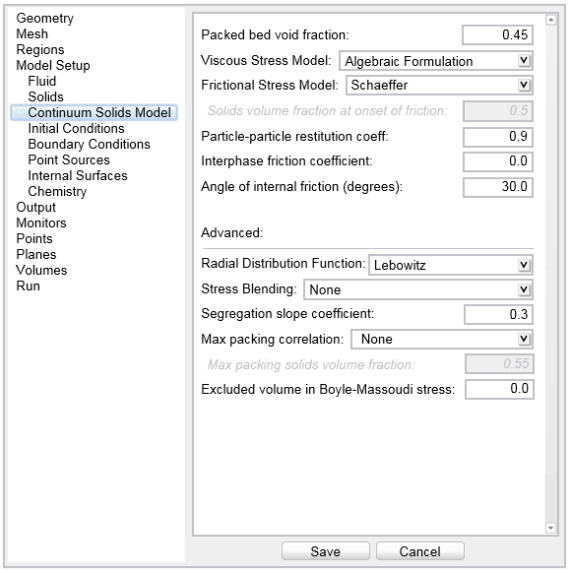
    - Sets keyword EPS_F_MIN
- Specify particle-particle restitution coefficient
    - Specification available only when required
    - Required for MMAX >=2
    - Required for viscous stress models except GHD and algebraic formulation
    - Sets keyword C_E
- Specify interphase friction coefficient
    - Specification available only when required
    - Required for MMAX >= 2
    - Sets keyword C_F
- Specify angle of particle-particle friction
    - Specification available only when required
    - Required for FRICTION_MODEL=SCHAEFFER
    - Required for FRICTION_MODEL=SRIVASTAVA
    - Sets keyword PHI

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

- Select radial distribution function
    - Selection always available
    - Available selections:
        - Carnahan-Starling
            - Only available for MMAX==1
            - Sets keyword RDF_TYPE to LEBOWITZ (this is correct)
        - *Lebowitz*
            - Only available for MMAX >1
            - Sets keyword RDF_TYPE to LEBOWITZ
        - *Mansoori*
            - Only available for MMAX>1
            - Sets keyword RDF_TYPE to MANSOORI
        - *Modified Lebowitz*
            - Only available for MMAX >1
            - Sets keyword RDF_TYPE to MODIFIED_LEBOWITZ
        - *Modified Mansoori*
            - Only available for MMAX>1
            - Sets keyword RDF_TYPE to MODIFIED_MANSOORI

- Select stress blending model
    - Selection only available with FRICTION_MODEL=SCHAEFFER
    - 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
        - *Sigmodial*
            - Selection always available
            - Sets keyword BLENDING_FUNCTION to SIGM_BLEND
- Specify the segregation slope coefficient
    - Only available for MMAX > 1 in conjunction with the following viscous stress models: algebraic formulation; Lun. 1984; Simonin, 1996; Ahmadi, 1995
    - Unavailable with (+other requirements)
    - Sets keyword SEGREGATION_SLOPE_COEFFICIENT

- Select maximum packing correlation
  - Selection only available with FRICTION_MODEL=SCHAEFFER and MMAX >1
  - 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 MMAX = 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*)
  - Only available with algebraic formulation of viscous stress model
  - 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
  - Enabled sets keyword GENER_PART_CONFIG to true
  - Disabled enables the user to specify number of entries in particle input file
    - Default value is 0
    - Sets keyword PARTICLES
- Select numerical integration method
  - Selection always available
  - Available selections
    - *Euler* [DEFAULT]
      - Selection always available
      - Sets keyword DES_INTG_METHOD to 'EULER'
    - *Adams-Bashforth*

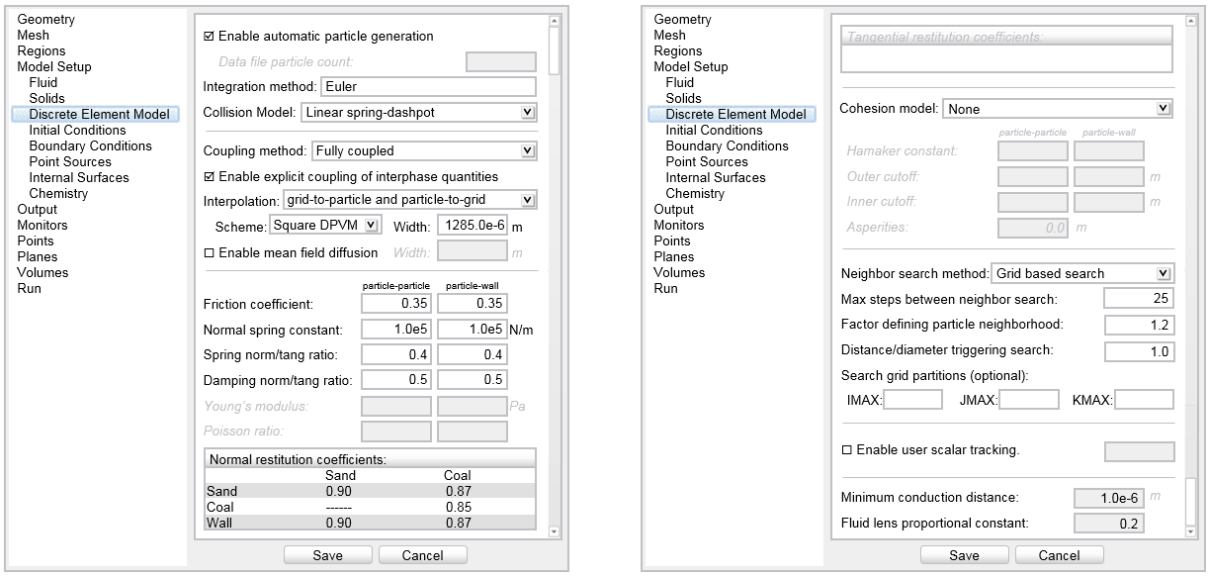
        - Selection always available
        - Sets keyword DES_INTG_METHOD to 'ADAMS_BASHFORTH'
- Selection collision model
    - Selection always available
    - Available selections
        - *Linear Spring-Dashpot* [DEFAULT]
            - Selection always available
            - Sets keyword DES_COLL_MODEL to 'LSD'
        - *Hertzian*
            - Selection always available
            - Sets keyword DES_COLL_MODEL to 'HERTZIAN'
- Select gas-solids coupling scheme:
    - Selection unavailable if fluid model is disabled
    - 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
    - *Unavailable for GARG_2012 interpolation*
- Select interpolation framework:
    - Selection always available
    - 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:
    - Selection available except when no-interpolation framework is selected
    - 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*)
    - Specification only available with SQUARE_DPVM interpolation scheme
    - Sets keyword DES_INTERP_WIDTH
- Option to enable diffusion of particle data

    - Selection unavailable with GARG_2012 interpolation scheme
    - No keyword is set by this option
    - Enables the user to specify a diffusion width
        - Sets keyword DES_DIFFUSE_WIDTH
- Specify friction coefficient
    - Specification always required
    - Sets keyword MEW (MEW_W)
- Specify normal spring constant
    - Only available for LSD collision model
    - Sets keyword KN (KN_W)
- Specify tangential spring constant factor
    - Only available for LSD collision model
    - Sets keyword KT_FAC (KT_W_FAC)
    - Default values of 2.0/7.0
- Specify tangential damping coefficient factor
    - Only available for LSD collision model
    - Sets keyword DES_ETAT_FAC (DES_ETAT_W_FAC)
    - Default values of 0.5
- Specify Young's modulus
    - Only available for Hertzian collision model
    - Sets keyword E_YOUNG (EW_YOUNG)
- Specify Poisson ratio:
  Only available for Hertzian collision model
    - Sets keyword V_POISSON (VW_POISSON)
- Specify normal restitution coefficient
    - Specification always required
    - Sets keyword DES_EN_INPUT (DES_EN_WALL_INPUT)
    - Input given as an upper triangular matrix
- Specify tangential restitution coefficient
    - Specification available for Hertzian collision model
    - Sets keyword DES_ET_INPUT (DES_ET_WALL_INPUT)
    - Input given as an upper triangular matrix
- Select cohesion model
    - Selection always available
    - 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
    - Specification only available for Van der Waals cohesion model
    - Sets keyword HAMAKER_CONSTANT (WALL_HAMAKER_CONSTANT)
- Specify outer cutoff;
    - Specification only available for Van der Waals cohesion model
    - Sets keyword VDW_OUTER_CUTOFF (WALL_OUTER_CUTOFF)
- Specify inner cutoff
    - Specification only available for Van der Waals cohesion model
    - Sets keyword VDW_INNER_CUTOFF (WALL_INNER_CUTOFF)
- Specify asperities
    - Specification only available for Van der Waals cohesion model

- Sets keyword ASPERITIES

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

- Select Neighbor Search Method
  - Selection always available
  - 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
  - Specification always available
  - Sets keyword NEIGHBOR_SEARCH_N
- Specify factor defining particle neighborhood
  - Specification always available
  - Sets keyword FACTOR_RLM
- Specify neighborhood search radius ratio
  - Specification always available
  - Sets keyword NEIGHBOR_SEARCH_RAD_RATIO
- Specify search grid partitions (optional)
  - Specification always available
  - Sets keyword DESGRIDSEARCH_IMAX
  - Sets keyword DESGRIDSEARCH_JMAX
  - Sets keyword DESGRIDSEARCH_KMAX
- Enable user scalar tracking
  - Selection always available
  - Does not directly set any keywords
  - Enables specification of number of user scalars
    - Sets keyword DES_USR_VAR_SIZE
- Define minimum distance for contact conduction (*optional*)
  - *Unavailable if not solving energy equations*
- Define fluid lens proportion constant (*optional*)
  - *Unavailable if not solving energy equations*

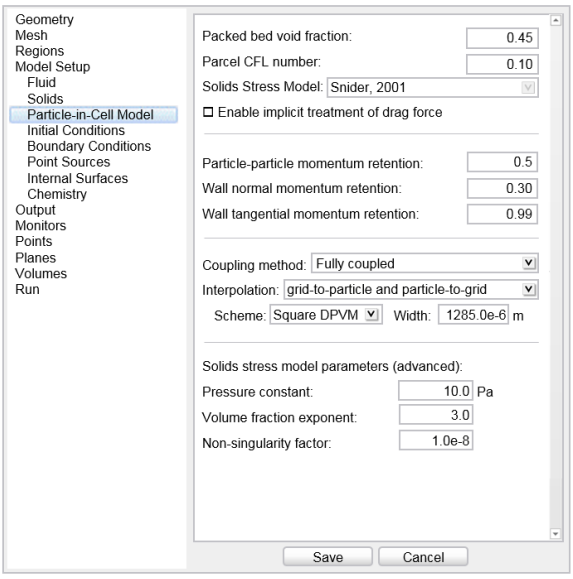


Mockup of Task pane for specifying the discrete element model parameters.

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

- Specify void fraction at close pack (*required*)
  - Sets keyword EP_STAR [0.42]
- Define parcel CFL number
  - Sets keyword CFL_PIC
  - DEFAULT value of 0.1
- Select solid stress model
  - Selection always available
  - Available selection
    - *Snider, 2001* [DEFAULT]
      - Selection always available
      - Sets keyword MPPIC_SOLID_STRESS_SNIDER=.T.
- Option to enable implicit treatment of drag force
  - Sets keyword: MPPIC_PDRAG_IMPLICIT
  - Disabled [DEFAULT]
- Define particle-particle momentum retention
  - Sets keyword MPPIC_COEFF_EN1
  - DEFAULT value of 0.4
- Define wall normal momentum retention
  - Sets keyword MPPIC_COEFF_EN_WALL
  - DEFAULT value of 0.3
- Define wall tangential momentum retention
  - Sets keyword MPPIC_COEFF_ET_WALL
  - DEFAULT value of 0.99
- Select gas-solids coupling scheme:
  - Selection unavailable if fluid model is disabled
  - 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:
    - Selection always available
    - 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:
    - Selection available except when no-interpolation framework is selected
    - 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*)
    - Specification only available with SQUARE_DPVM interpolation scheme
    - Sets keyword DES_INTERP_WIDTH
- Define solids stress model parameter: pressure constant
    - Sets keyword PSFAC_FRIC_PIC
    - DEFAULT value of 10.0
- Define solids stress model parameter: volume fraction exponent
    - Sets keyword FRIC_EXP_PIC
    - DEFAULT value of 3.0
- Define solids stress model parameter: non-singularity factor
    - Sets keyword FRIC_NON_SING_FAC
    - DEFAULT value of 1.0E-8



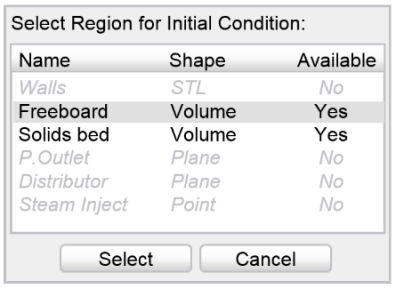
Mockup of Task pane for specifying the particle in cell model parameters.

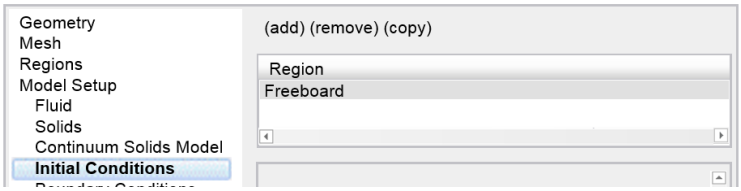
Initial Conditions Task Pane Window: This section allows a user to define the initial conditions for the described model. This section relies on regions named in the Regions section.

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 MFIX IC indices on the back end could get messy, and if so, scrap this idea.





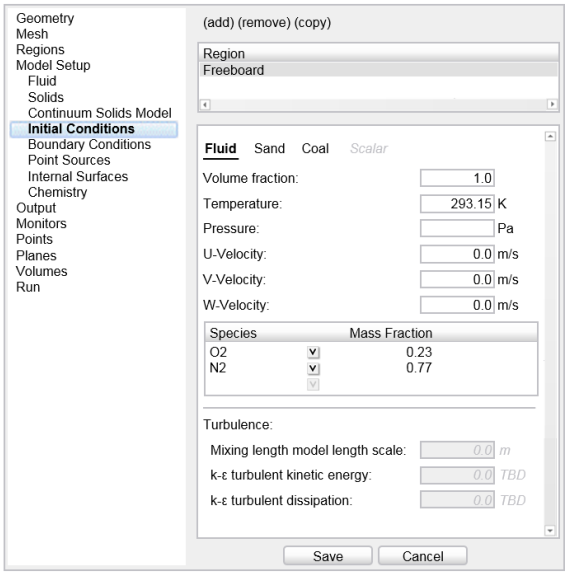
Tabs group initial condition parameters for phases and additional equations. Tabs are unavailable if no input is required from the user.

- 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
  - Specification never available
  - Sets keyword IC_EP_G(#)
  - CALCULATED from 1.0 - sum(IC_EP_s(#,#)
  - GUI should show the result of the calculation.
- Define temperature
  - Specification always available
  - Input required for any of the following
    - Fluid density model: Ideal Gas Law
    - Fluid viscosity model: Sutherland's Law
    - Energy equations are solved
  - Sets keyword IC_T_G(#)
  - DEFAULT value of 293.15
- Define pressure (*optional*)
  - Specification always available
  - Sets keyword IC_P_g(#)
  - DEFAULT - no input-
- Define velocity components (*required*)
  - Specification always available
  - Sets keywords IC_U_G(#), IC_V_G(#), IC_W_G(#)
  - DEFAULT value of 0.0
- Select species and set mass fractions (table format)
  - Specification always available
  - Sets keyword IC_X_G
  - Input required for species equations
  - Drop down menu of fluid species
  - DEFAULT - last defined species has mass fraction of 1.0
  - Error check: mass fractions must sum to one
- Turbulence: Define mixing length model length scale
  - Specification only available with Mixing Length turbulence model
  - Sets keyword IC_L_SCALE(#)
  - DEFAULT value of 1.0
- Turbulence: Define k-ε turbulent kinetic energy
  - Specification only available with K-Epsilon turbulence model
  - Sets keyword IC_K_TURB_G(#)
  - DEFAULT value of 0.0
- Turbulence: Define k-ε turbulent dissipation
  - Specification only available with K-Epsilon turbulence model
  - Sets keywords IC_E_TURB_G(#)
  - DEFAULT value of 0.0
- Advanced: Define radiation coefficient
  - Specification only available when solving energy equations
  - Sets keyword IC_GAMA_RG(#)
  - DEFAULT value of 0.0
- Advanced: Define radiation temperature

- Specification only available when solving energy equations
- Sets keyword IC_T_RG(#)
- DEFAULT value of 293.15

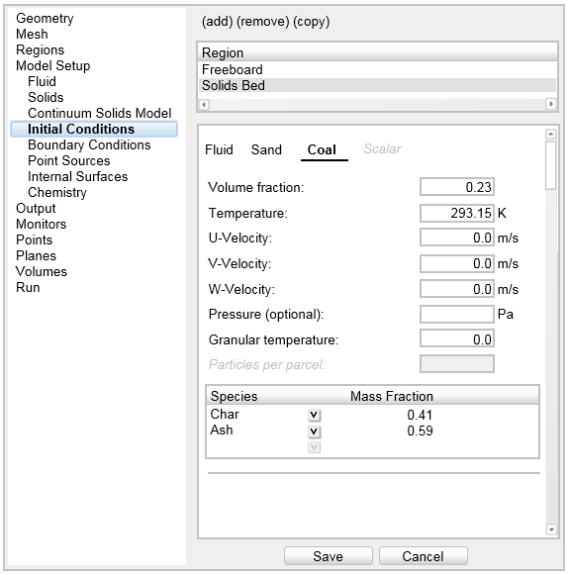


Mockup of Task pane for specifying the fluid properties for initial conditions parameters.

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

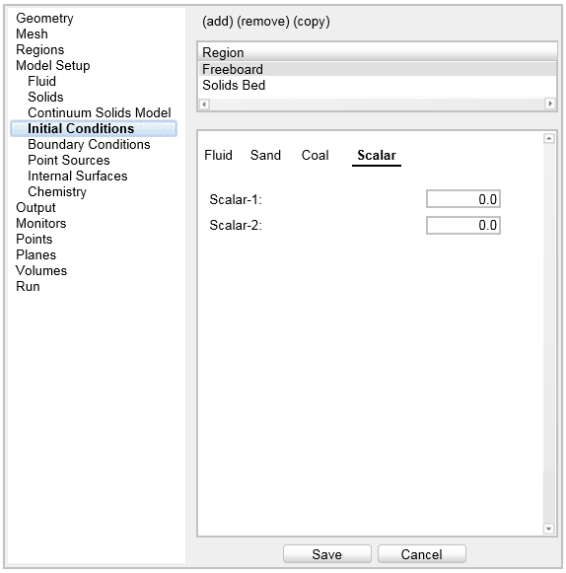
- Define volume fraction (*required*)
  - Specification always available
  - Sets keyword IC_EP_S(#,#)
  - DEFAULT value of 0.0
  - Some input decks may or may not contain IC_EP_S keyword:
    - Volume fraction is specified using the solids bulk density
      - IC_EP_S(#,#) == IC_ROP_S(#,#) / IC_ROs(#)
      - Solids density IC_ROs is determined by the solids density model. For constant solids density, use RO_S0. For variable solids density, see "Calculating Variable Solids Density" section in the appendix.
    - 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
  - Specification always available
  - Input required when solving energy equations
  - Sets keyword IC_T_S(#,#)
  - DEFAULT value of 293.15
- Define velocity components (*required*)
  - Specification always available
  - Sets keywords IC_U_S(#,#), IC_V_S(#,#), IC_W_S(#,#)
  - DEFAULT value of 0.0
- Define pressure (*optional*)
  - Specification only available for SOLIDS_MODEL(#)='TFM'
  - Sets keyword IC_P_STAR(#)
  - DEFAULT of 0.0
  - Common to all phases - Warn user if changed.
- Define granular temperature

    - 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'
    - Sets keyword IC_THETA_M(#,#)
    - DEFAULT value of 0.0
- Define particles per parcel
    - Specification only available for SOLIDS_MODEL(#)='PIC'
    - Sets keyword IC_PIC_CONST_STATWT(#,#)
    - DEFAULT value of 10.0
- Select species and set mass fractions (table format)
    - Specification always available
    - Input required for species equations
    - Drop down menu of solids species
    - Sets keyword IC_X_S(#,#,#)
    - DEFAULT - last defined species has mass fraction of 1.0
    - Error check: mass fractions must sum to one
- Advanced: Option to enable fitting DES particles to region
    - Option only available for DEM solids
    - Sets keyword: IC_DES_FIT_TO_REGION
    - Disabled [DEFAULT]
- Advanced: Define radiation coefficient
    - Specification only available when solving energy equations
    - Sets keyword IC_GAMA_RS(#,#)
    - DEFAULT value of 0.0
- Advanced: Define radiation temperature
    - Specification only available when solving energy equations
    - Sets keyword IC_T_RS(#,#)
    - DEFAULT value of 293.15



Mockup of Task pane for specifying solids-# initial condition parameters.
Scalar (tab) - *Tab only available if scalar equations are solved*

- Define initial scalar value
    - Sets keyword IC_SCALAR(#,#)
    - DEFAULT value of 0.0



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*

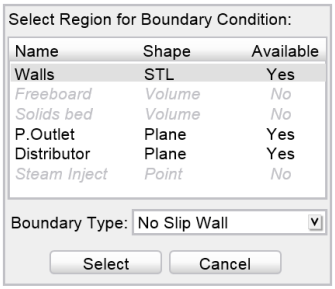
- Volume and plane regions set keyword BC_TYPE(#) to 'PSW'
- STL regions set keyword BC_TYPE(#) to 'CG_PSW'

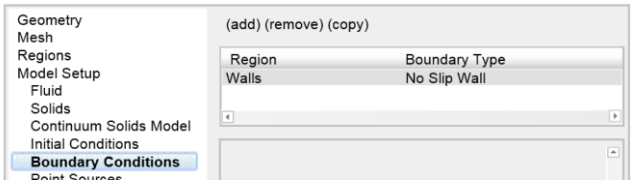
▪ *Pressure Inflow*
- Plane regions set keyword BC_TYPE(#) to 'PI'
- Not available for volume regions
- Not available for STL regions

▪ *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

o Specification always available
o DEFAULT - No slip wall
o 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.

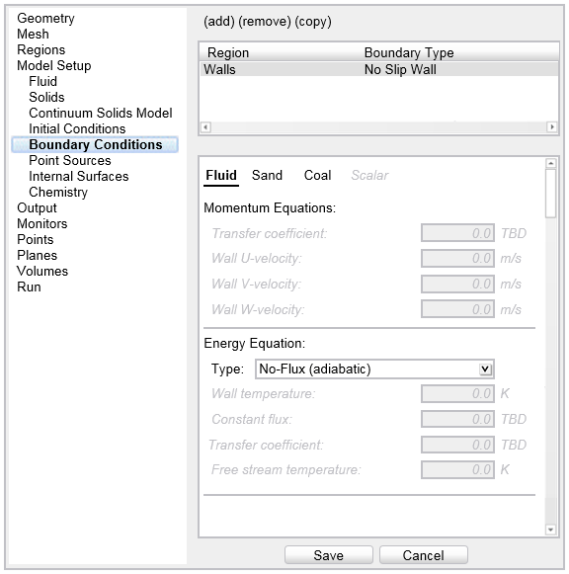
Subtask Pane Tab for Wall type (NSW, FSW, PSW, CG_NSW, CG_FSW, CG_PSW) Boundary Condition Regions

Fluid (tab)

- Define transfer coefficient
  - Specification only available with PSW
  - Sets keyword BC_HW_G(#)
  - DEFAULT value of 0.0
- Define Wall U-velocity
  - Specification only available with PSW
  - Sets keyword BC_UW_G(#)
  - DEFAULT value of 0.0
- Define Wall V-velocity
  - Specification only available with PSW
  - Sets keyword BC_VW_G(#)
  - DEFAULT value of 0.0

- Define Wall W-velocity
  - Specification only available with PSW
  - Sets keyword BC_WW_G(#)
  - DEFAULT value of 0.0
- Select energy equation boundary type:
  - Selection only available when solving energy equations
  - 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
  - Specification only available with *'Specified Temperature*' BC type
  - Sets keyword BC_TW_G(#)
  - DEFAULT value of 293.15
- Define constant flux
  - Specification only available with *'Specified Flux*' BC type
  - Sets keyword BC_C_T_G(#)
  - DEFAULT value of 0.0
- Define transfer coefficient
  - Specification only available with *'Convective Flux*' BC type
  - Sets keyword BC_HW_T_G(#)
  - DEFAULT value of 0.0
- Define free stream temperature
  - Specification only available with *'Convective Flux*' BC type
  - Sets keyword BC_TW_G(#)
  - DEFAULT value of 0.0
- Select species equation boundary type:
  - Selection only available when solving species equations
  - 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
    - Specification only available with *'Specified Mass Fraction*' BC type
    - Sets keyword BC_XW_G(#)
    - DEFAULT value of 0.0
- Define constant flux
    - Specification only available with *'Specified Flux*' BC type
    - Sets keyword BC_C_X_G(#)
    - DEFAULT value of 0.0
- Define transfer coefficient
    - Specification only available with *'Convective Flux*' BC type
    - Sets keyword BC_HW_X_G(#)
    - DEFAULT value of 0.0
- Define free stream mass fraction
    - Specification only available with *'Convective Flux*' BC type
    - Sets keyword BC_XW_G(#)
    - 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
    - Disabled for DEM and PIC solids
    - Disabled (0.0) for CARTESIAN_GRID = .TRUE.
    - Disabled (0.0) for KT_TYPE = 'ALGEBRAIC'
    - Disabled (0.0) for KT_TYPE = 'GHD_2007'
    - Sets keyword BC_JJ_PS(#)

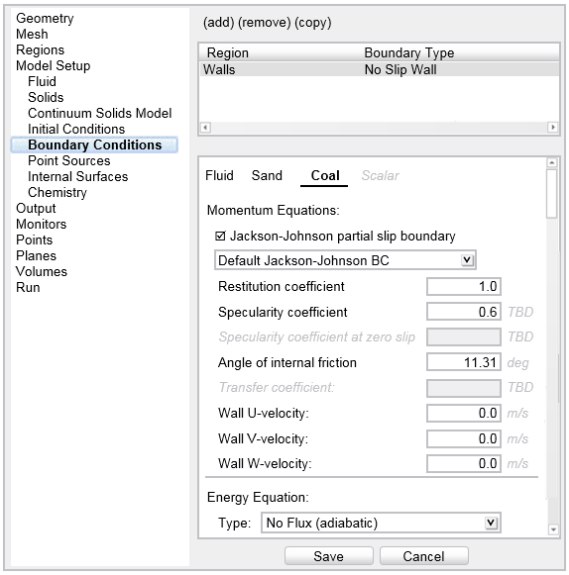
    - DEFAULT value of 1.0 when not disabled
- Select type of Jackson and Johnson BC:
    - Disabled for DEM and PIC solids
    - Selection only available BC_JJ_PS(#) = 1.0
    - Available selections:
        - *Default Jackson-Johnson BC* [DEFAULT]
            - Sets keyword BC_JJ_M to .FALSE.
            - Sets keyword JENKINS to .FALSE.
        - *Variable specularity 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
    - Disabled for DEM and PIC solids
    - Specification only available with BC_JJ_PS(#) = 1.0
    - Sets keyword E_W
    - DEFAULT value of 1.0
    - Required when available
- Define specularity coefficient
    - Disabled for DEM and PIC solids
    - Specification only available with BC_JJ_PS(#)=1.0 and JENKINS=.FALSE.
    - Sets keyword PHIP
    - DEFAULT value of 0.6
    - Required when available
- Define specularity coefficient at zero slip
    - Disabled for DEM and PIC solids
    - Specification only available with BC_JJ_PS(#)=1.0 and BC_JJ_M=.TRUE.
    - Sets keyword PHIP0
    - DEFAULT -blank-
    - Optional when available
- Define angle of internal friction
    - Disabled for DEM and PIC solids
    - Sets keyword PHI_W
    - Specification only available with BC_JJ_PS(#)=1.0 and (JENKINS=.TRUE. FRICTION_MODEL=SRIVASTAVA)
    - DEFAULT value of 11.31
    - Required when available
- Define transfer coefficient
    - Disabled for DEM and PIC solids
    - Specification only available with PSW
    - Sets keyword BC_HW_S(#,#)
    - DEFAULT value of 0.0
- Define Wall U-velocity
    - Disabled for DEM and PIC solids
    - Specification only available with PSW or BC_JJ_PS(#) = 1.0
    - Sets keyword BC_UW_S(#,#)
    - DEFAULT value of 0.0
- Define Wall V-velocity
    - Disabled for DEM and PIC solids
    - Specification only available with PSW or BC_JJ_PS(#) = 1.0
    - Sets keyword BC_VW_S(#,#)
    - DEFAULT value of 0.0

- Define Wall W-velocity
  - Disabled for DEM and PIC solids
  - Specification only available with PSW or BC_JJ_PS(#) = 1.0
  - Sets keyword BC_WW_S(#,#)
  - DEFAULT value of 0.0
- Select energy equation boundary type:
  - Disabled for PIC solids
  - Selection only available when solving energy equations
  - 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
  - Disabled for PIC solids
  - Specification only available with *'Specified Temperature*' BC type
  - Sets keyword BC_TW_S(#,#)
  - DEFAULT value of 293.15
- Define constant flux
  - Disabled for PIC solids
  - Specification only available with *'Specified Flux*' BC type
  - Sets keyword BC_C_T_S(#,#)
  - DEFAULT value of 0.0
- Define transfer coefficient
  - Disabled for PIC solids
  - Specification only available with *'Convective Flux*' BC type
  - Sets keyword BC_HW_T_S(#,#)
  - DEFAULT value of 0.0
- Define free stream temperature
  - Disabled for PIC solids
  - Specification only available with *'Convective Flux*' BC type
  - Sets keyword BC_TW_S(#,#)
  - DEFAULT value of 0.0
- Select granular energy equation boundary type:
  - Disabled for DEM and PIC solids
  - Selection only available with BC_JJ_PS(#)=0.0 and KT_TYPE /= 'ALGEBRAIC'
  - 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_THETAW_M(#,#) to UNDEFINED

    - *Specified Temperature*
        - Sets keyword BC_HW_THETA_M(#,#) to UNDEFINED
        - Sets keyword BC_C_THETA_M(#,#) to 0.0
        - Requires BC_THETAW_M(#,#)
    - *Specified Flux*
        - Sets keyword BC_HW_THETA_M(#,#) to 0.0
        - Requires BC_C_THETA_M(#)
        - Sets keyword BC_THETAW_M(#,#) to UNDEFINED
- Define granular temperature
    - Disabled for DEM and PIC solids
    - Specification only available with *'Specified Temperature*' BC type
    - Sets keyword BC_THETAW_M(#,#)
    - DEFAULT value of 0.0
- Define constant flux
    - Disabled for DEM and PIC solids
    - Specification only available with *'Specified Flux*' BC type
    - Sets keyword BC_C_THETA_M(#,#)
    - 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

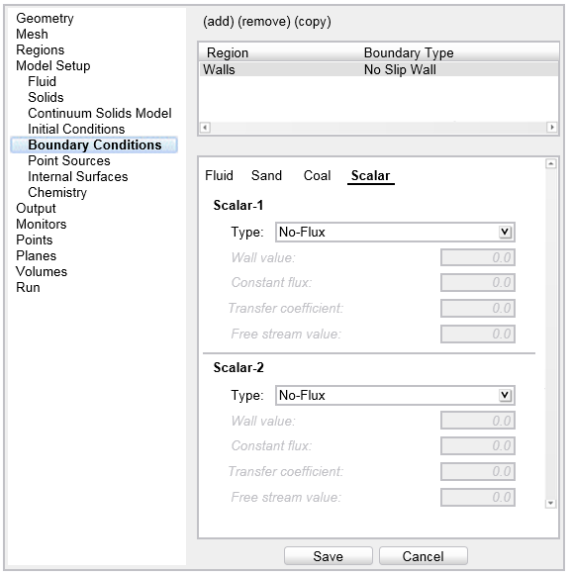


Mockup of Task pane for specifying the Solid-# properties for WALL boundary condition regions.

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

- Select scalar boundary type:
    - 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
    - Specification only available with *'Specified Temperature*' BC type
    - Sets keyword BC_SCALARW (#,#)
    - DEFAULT value of 0.0
- Define constant flux
    - Specification only available with *'Specified Flux*' BC type
    - Sets keyword BC_C_SCALAR (#,#)
    - DEFAULT value of 0.0
- Define transfer coefficient
    - Specification only available with *'Convective Flux*' BC type
    - Sets keyword BC_HW_SCALAR(#,#)
    - DEFAULT value of 0.0
- Define free stream temperature
    - Specification only available with *'Convective Flux*' BC type
    - Sets keyword BC_SCALARW (#,#)
    - 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)

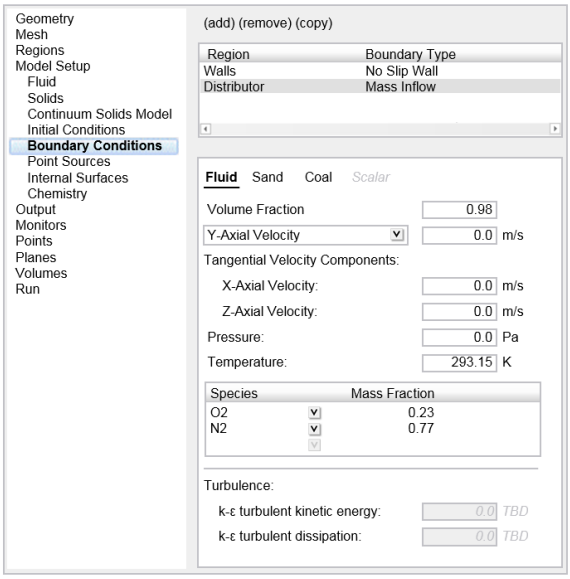
- Define volume fraction
  - Specification always available
  - Sets keyword BC_EP_G(#)
    - DEFAULT value of 1.0 for MI and CG_MI; leave [UNDEFINED] for PI
    - Error Check: For MI and CG_MI, BC_EP_G(#) + BC_EP_S(#,:) = 1.0
    - Error Check: For PI - either all are defined and sum to 1, or all are undefined
- Define inflow properties: *Mass inflow specification changes based on the BC_TYPE and Region orientation (e.g., XZ-Plane)*
  - ***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^3/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
  - ***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^3/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
  - ***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^3/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

- ***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
  - Specification always available
  - Input required for any of the following
    - Fluid density model: Ideal Gas Law
    - Fluid viscosity model: Sutherland's Law
    - Energy equations are solved
  - Sets keyword BC_T_G(#)
  - DEFAULT value of 293.15
- Define pressure
  - Specification always available
  - Input required when combining ideal gas law and specified mass inflow rate
  - Input required for BC_TYPE = PI
  - Sets keyword BC_P_G(#)
  - DEFAULT 101.325d3
- Select species and set mass fractions (table format)
  - Specification always available
  - Input required for species equations
  - Drop down menu of fluid species
  - Sets keyword BC_X_G(#,#)
  - DEFAULT - last defined species has mass fraction of 1.0
  - Error check: mass fractions must sum to one
- Turbulence: Define k-ε turbulent kinetic energy
  - Specification only available with K-Epsilon turbulence model
  - Sets keyword BC_K_TURB_G(#)
  - DEFAULT value of 0.0
- Turbulence: Define k-ε turbulent dissipation
  - Specification only available with K-Epsilon turbulence model
  - Sets keywords BC_E_TURB_G(#)
  - DEFAULT value of 0.0



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

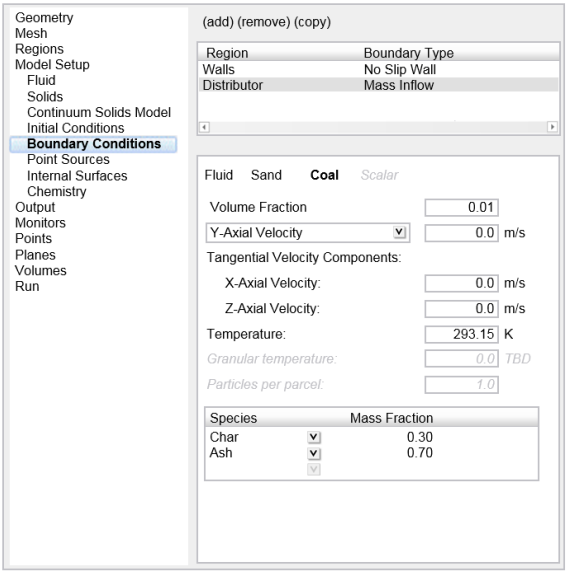
Solid-# (tab) - *Rename tab to user provided solids name.*

- Define volume fraction
  - Specification always available
  - 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 the solids density model. For constant solids density, use RO_S0. For variable solids density, see "Calculating Variable Solids Density" section in the appendix.
      - 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)*
  - ***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^3/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

- ***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^3/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
- ***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^3/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
- ***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
    - Specification always available
    - Input required when energy equations are solved
    - Sets keyword BC_T_S(#,#)
    - DEFAULT value of 293.15
- Select species and set mass fractions (table format)
    - Specification always available
    - Input required for species equations
    - Drop down menu of solid species
    - Sets keyword BC_X_S(#,#,#)
    - DEFAULT - last defined species has mass fraction of 1.0
    - Error check: mass fractions must sum to one



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(#,#)
  - Error check: if specified, mass fractions must sum to one_

Solids-# (tab)

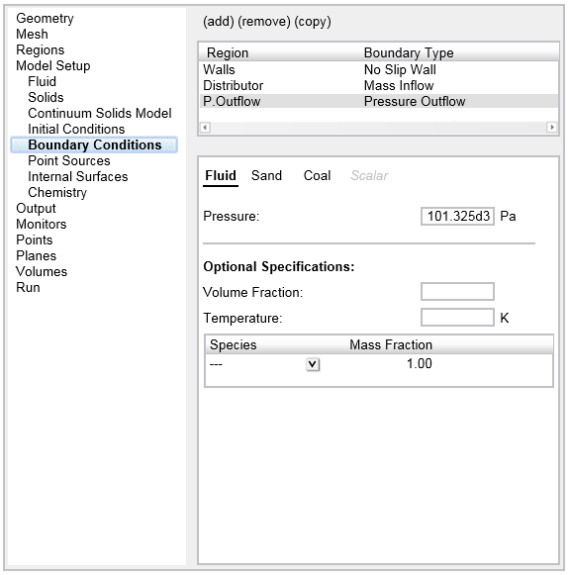
All inputs are optional. They do not have default values, because MFIX will calculate appropriate values if they are unspecified and 'backflow' occurs at the outlet.

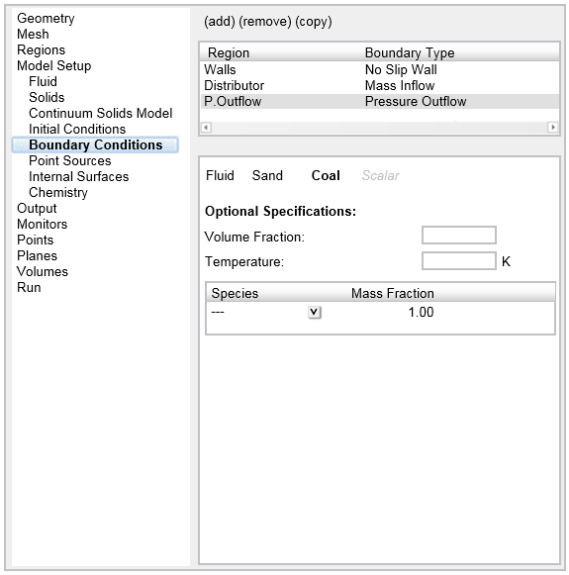
- Define volume fraction
  - Specification always available
  - Sets keyword BC_EP_S(#,#)
  - No DEFAULT value
  - Error Check: If any volume fraction for the BC region is specified, then all volume fractions for the BC region must be specified and must sum to one.
- Define temperature
  - Specification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





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)*
  - ***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^3/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
  - ***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^3/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
- ***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^3/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
- ***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.
  - Specification always available
  - Input required
  - Sets keyword BC_DT_0(#)
  - DEFAULT value of 0.1
  - 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 '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: MFIX allows some strange 'partially' defined volume fractions for mass outflows but these will not be supported within the GUI.

- Define volume fraction
  - Specification required for specified mass or volumetric flowrates.
  - Input required
  - Sets keyword BC_EP_G(#)
  - DEFAULT value 1.0
  - 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 is required when solving the energy equations (ENERGY_EQ == .TRUE.) or with mass or volumetric flowrates and (RO_G0 == UNDEFINED)
  - DEFAULT value 293.15
  - Sets keyword BC_T_G(#)
- Select species and set mass fractions (table format)
  - Specification is available with mass or volumetric flowrates when (R_G0 == UNDEFINED)
  - DEFAULT value 1.0 of last defined species
  - Sets keyword BC_X_G(#,#)
  - Error check: if specified, mass fractions must sum to one_

Solids-# (tab)

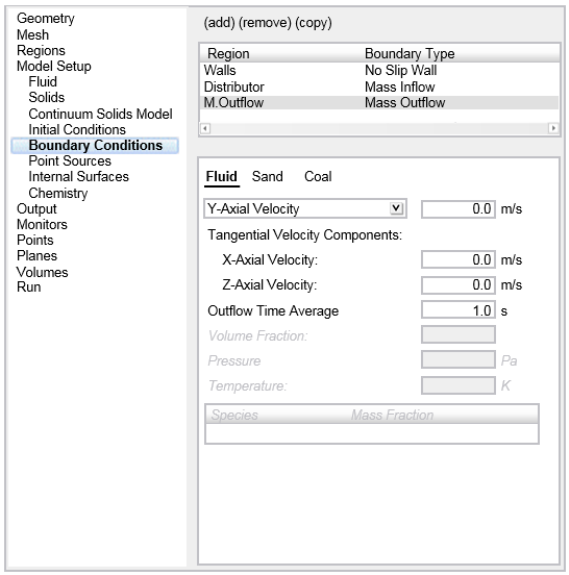
- Define outflow properties: *Mass outflow specification changes based on the BC_TYPE and Region orientation (e.g., XZ-Plane)*
  - ***For BC_TYPE='MO' and XZ-Plane region***
    - Select mass outflow specification type:
      - Available selections:
      - *Y-Axial Velocity (m/s)* [DEFAULT]
        - Sets keyword BC_V_S(#,#)
        - DEFAULT value of 0.0
      - *Volumetric Flowrate (m^3/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(#,#)

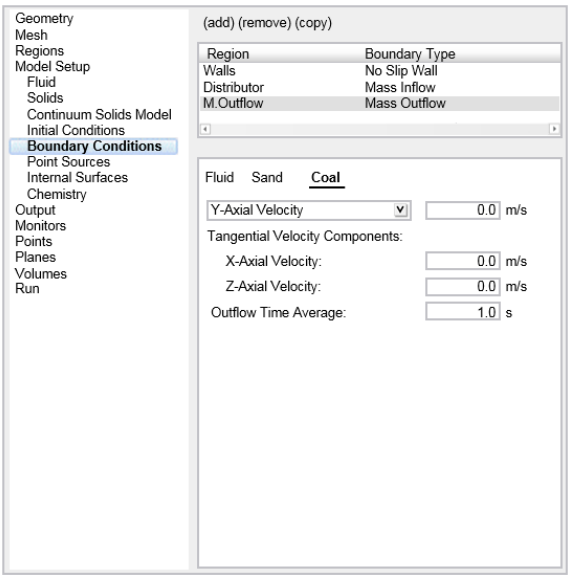
        - DEFAULT value of 0.0
- ***For BC_TYPE='MO' and YZ-Plane region***
    - Select mass outflow specification type:
        - Available selections:
        - *X-Axial Velocity (m/s)* [DEFAULT]
            - Sets keyword BC_U_S(#,#)
            - DEFAULT value of 0.0
        - *Volumetric Flowrate (m^3/s)*
            - 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
- ***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^3/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
- ***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.
    - Specification always available
    - Input required

- Sets keyword BC_DT_0(#)
- DEFAULT value of 0.1
- 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 messing indicating that this value is 'constant' across all phases should be given.

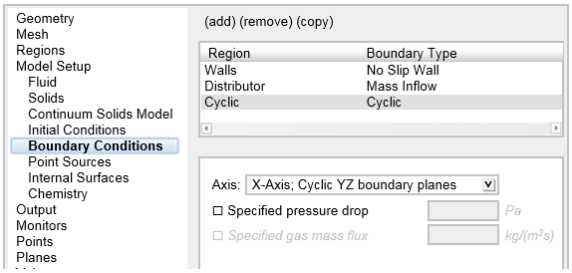




Subtask Pane Tab for Cyclic type Boundary Conditions

- Select cyclic axis
  - 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
  - DEFAULT value of .FALSE.
  - 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
  - Error check: Only one axis can have a specified pressure drop
  - 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

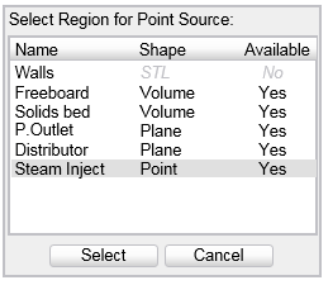
- Requires specified pressure drop
- Sets keyword FLUX_G
- DEFAULT value of 0.0
- Error check: Only one axis can have a specified mass flux. (This should not be an issue as it requires a specified pressure drop which can only be applied to one axis.)

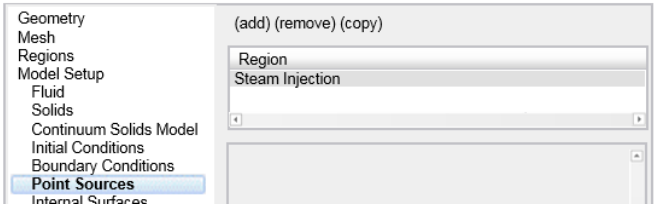


Point Source Task Pane Window: This section allows a user to define point sources for the described model. This section relies on regions named in the Regions section.

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:

- Select mass inflow specification type:
- Sets keyword PS_MASSFLOW_S(#,#)
- DEFAULT value of 0.0

- Define temperature
    - Specification only available when solving energy equations
    - DEFAULT value 293.15
    - Sets keyword PS_T_S(#,#)
- 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_S(#,#,#)
    - Error check: if specified, mass fractions must sum to one
- Define X-axial velocity:
    - Specification always
    - No DEFAULT value (blank)
    - Sets keyword PS_U_S(#,#)
- Define Y-axial velocity:
    - Specification always
    - No DEFAULT value (blank)
    - Sets keyword PS_V_S(#,#)
- Define Z-axial velocity:
    - Specification always
    - No DEFAULT value (blank)
    - Sets keyword PS_W_S(#,#)

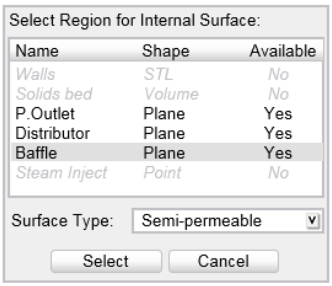
Internal Surfaces Task Pane Window: This section allows a user to define internal surfaces for the described model. This section relies on regions named in the Regions section.

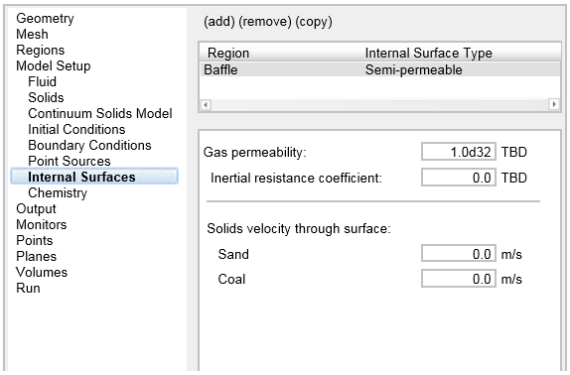
The top of the task pane is where users define/select IS regions

- 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:
    - Specification only available for semipermeable regions
    - DEFAULT value 1.0d32
    - Sets keyword IS_PC(#,1)
- Internal resistance coefficient:
    - Specification only available for semipermeable regions
    - DEFAULT value 0.0
    - Sets keyword IS_PC(#,2)
- Solids velocity through surface:
    - Specification only available for semipermeable regions
    - DEFAULT value 0.0
    - Sets keyword IS_VEL_s(#,PHASE)
    - *There should be a line for each solids phase. Use the user provided solids name.*



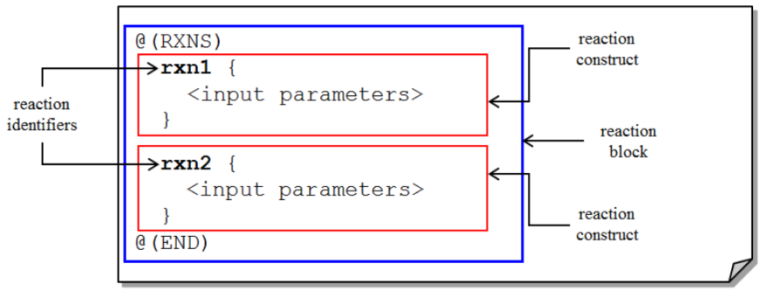


Chemistry Task Pane Window: This section allows a user to define chemical reaction input.

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

- Enable the stiff chemistry solver
  - Selection always available
  - Sets keyword STIFF_CHEMISTRY to .TRUE.

Chemical reaction input is handled different that 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 identify.

- Specify the reaction identifier (Name)
  - Specification always available
  - DEFAULT value reactionN (for the Nth reaction)
  - Reaction identifiers must be "Fortran compilable"
    - Alphanumeric combinations (no special characters excluding underscores)

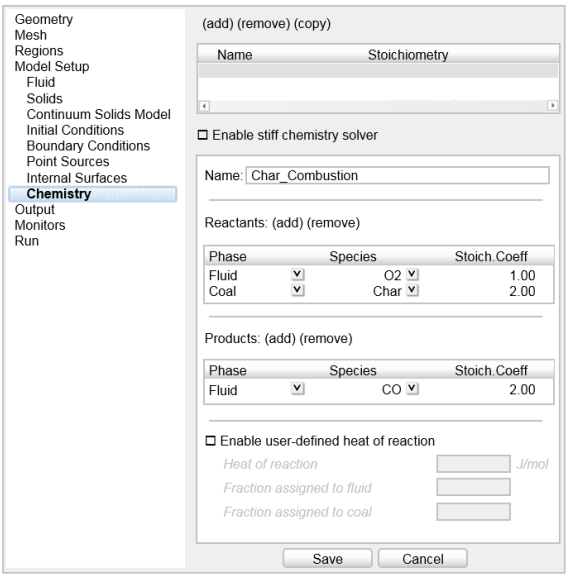
        - Limited to 32 characters
        - First character must be a letter
        - No black spaces
- Specify chemical reaction reactants (table format)
    - Use +/- buttons to add/remove reactants
    - Column 1 - Select phase for reactant
        - Use drop down list of user defined phase names
        - 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)
    - 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
    - Column 3 - Enter stoichiometric coefficient
        - Numerical value (integer or float)
        - Value must be non-negative
- Specify chemical reaction products (table format)
    - Use +/- buttons to add/remove products
    - 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)
    - 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
    - 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.
    - Sets reaction construct keyword CHEM_EQ
    - Example: CHEM_EQ = "rcoeff1*reactant1 + rcoeff2*reactant2 --> pcoeff1*product1"

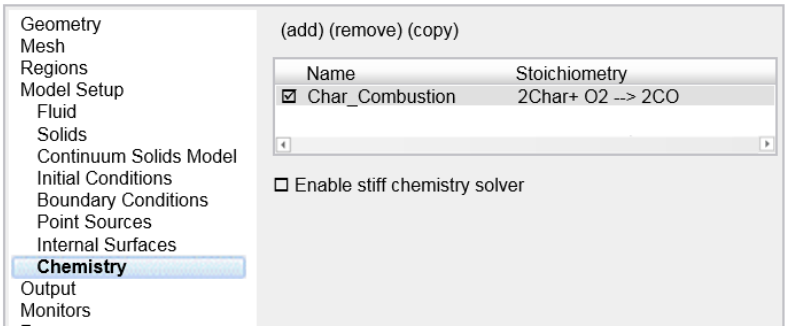
Error check: Mass of the reactants equal mass of the products (within a tolerance, 1.0e-6).
abs[(rcoeff1*MW(reactant1) + rcoeff2*MW(reactant2) - (pcoeff1*product1)] < 1.0e-6

- Enable user-defined heat of reaction
    - Selection always available
    - DEFAULT disabled
- Specify heat of reaction
    - Only available if user-defined heat of reaction is enabled
    - DEFAULT value 0.0
    - Sets reaction construct keyword DH
- Specify HoR fraction assigned to -phase-
    - Only available if user-defined heat of reaction is enabled
    - Homogeneous chemical reactions
        - Specification is not available
        - Set reaction construct keyword fracDH(#) to 1.0 where # is the phase index
    - 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



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."



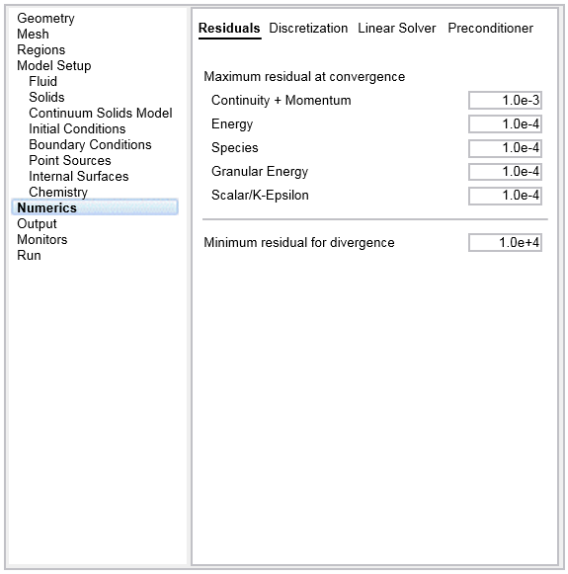
Numerics Task Pane Window:

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
  - Specification always available
  - Sets keyword TOL_RESID
  - DEFAULT value of 1.0e-3
- Specify residual for energy equations
  - Specification always available
  - Sets keyword TOL_RESID_T
  - DEFAULT value of 1.0e-4

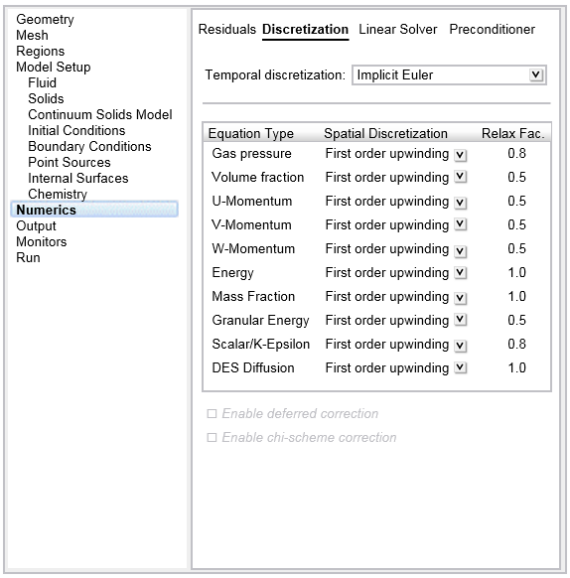
- Specify residual for species equations
  - Specification always available
  - Sets keyword TOL_RESID_X
  - DEFAULT value of 1.0e-4
- Specify residual for granular energy equations
  - Specification always available
  - Sets keyword TOL_RESID_TH
  - DEFAULT value of 1.0e-4
- Specify residual for scalar/K-Epsilon
  - Specification always available
  - Sets keyword TOL_RESID_SCALAR
  - DEFAULT value of 1.0e-4



Discretization (tab)

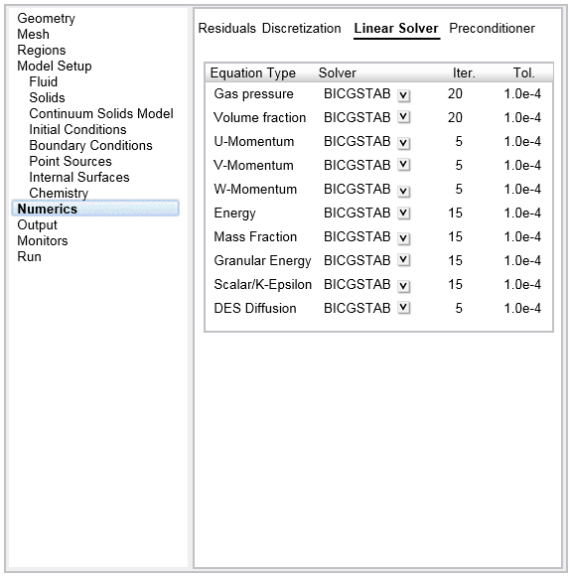
- Select temporal discretization scheme
  - Selection always available
  - Available selections:
    - *Implicit Euler* [DEFAULT]
      - Sets keyword CN_ON to .FALSE.
    - Crank-Nicholson
      - Sets keyword CN_ON to .TRUE.
- Specify spatial discretization and under relation factors (table format)
  - Specification always available
  - Column 1: List of equations
  - 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
- 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
    - Selection only available if minval(discretize) > 0
    - Sets keyword DEF_COR
    - DEFAULT value .FALSE.
- Enable chi-scheme correction
    - Selection only available if the species equation spatial discretization is SMART or MUSCL (DISCRETIZE(7) = 3 or 6)
    - Sets keyword CHI_SCHEME
    - DEFAULT value .FALSE.



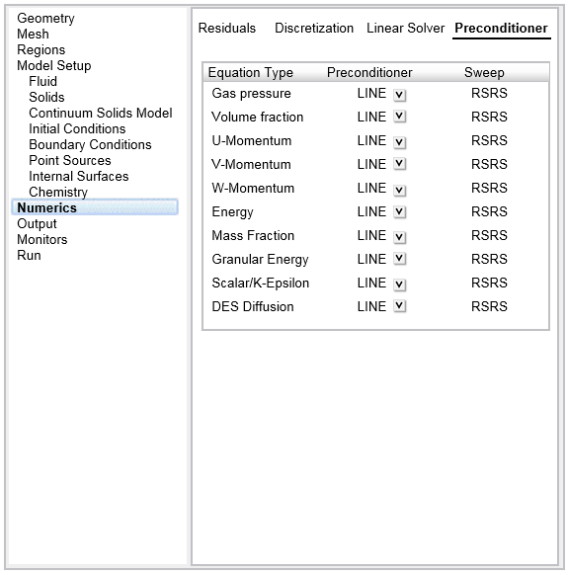
Linear Solver (tab)

- Specify linear solver, number of iterations, and convergence tolerance (table format)
  - Specification always available
  - Column 1: List of equations
  - 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
  - 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
  - Column 4: Specify convergence tolerance
    - Specification always available
    - Sets keyword LEQ_TOL
    - DEFAULT value of 1.0E-4 for all equations



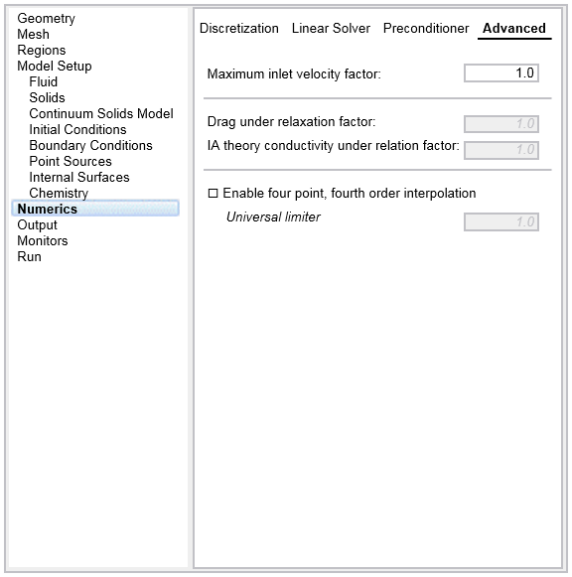
Preconditioner (tab)

- Specify linear solver, number of preconditioner and sweep direction (table format)
  - Specification only available for equations using BiCGSTAB solver
  - Column 1: List of equations
  - 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'
  - 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_SWEEP(#) to 'RSRS'
      - *All sweep*
        - Sets keyword LEQ_SWEEP(#) to 'ASAS'
      - *I-sweep*
        - Sets keyword LEQ_SWEEP(#) to 'ISIS'
      - *J-sweep*
        - Sets keyword LEQ_SWEEP(#) to 'JSJS'
      - *K-sweep*
        - Sets keyword LEQ_SWEEP(#) to 'KSKS'



Advanced (tab)

- Specify maximum inlet velocity factor
  - Specification always available
  - Sets keyword MAX_INLET_VEL_FAC
  - DEFAULT value of 1.0
  - Error check: Value greater than or equal to 1.0
- Specify drag under relation factor
  - Specification only available with MFIX-TFM and MFIX-Hybrid solvers
  - Sets keyword UR_F_GS
  - DEFAULT value of 1.0
  - Error check: Value bounded between 0 and 1
- Specify IA theory conductivity under relation factor
  - Specification only available with KT_TYPE = 'IA_NONEP'
  - Sets keyword UR_KTH_SML
  - DEFAULT value of 1.0
  - Error check: value bounded between 0 and 1
- Enable four point, fourth order interpolation
  - Specification always available
  - Sets keyword FPFOI
  - DEFAULT value of .FALSE.
- Specify the universal limiter
  - Specification only available if four point, forth order interpolation is enabled
  - Sets keyword C_FAC
  - DEFAULT value of 1.0
  - Error check: value bounded between 0 and 1



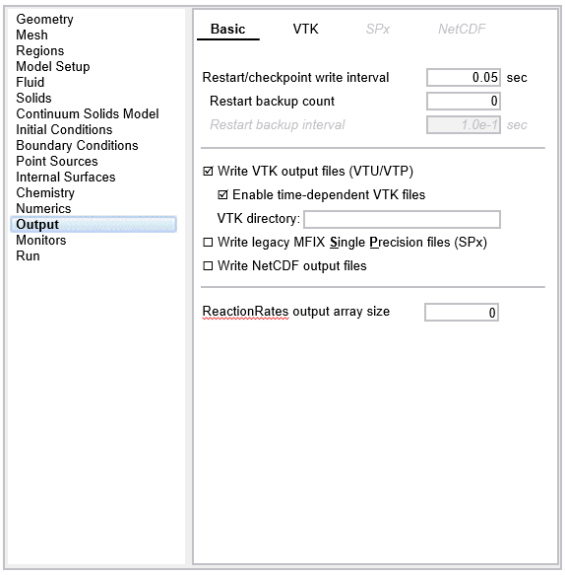
Output Task Pane Window:

The output input is split into tabs.

Basic (tab)

- Specify Restart/checkpoint write interval
  - Specification always available (required)
  - Sets keyword RES_DT
  - DEFAULT value of 1.0
- Specify the number of backup copies
  - Specification always available
  - Sets keyword RES_BACKUPS
  - DEFAULT value of 0
  - Error check: value is greater than or equal to 0
- Specify the backup interval
  - Specification only available if RES_BACKUPS > 0
  - Sets keyword RES_BACKUP_DT
  - DEFAULT value of 1.0
  - Error check: value must be greater than or equal to RES_DT
- Enable VTK output
  - Specification always available
  - Sets keyword WRITE_VTK_FILES
  - DEFAULT value of .FALSE.
  - Enables VTK tab
- Enable time-dependent VTK files
  - Specification only if WRITE_VTK_FILES = .TRUE.
  - Sets keyword TIME_DEPENDENT_FILENAME
  - DEFAULT value .TRUE.
- Specify VTK Directory
  - Specification only if WRITE_VTK_FILES = .TRUE.

    - Sets keyword VTU_DIR
    - No default (empty string)
- Write binary **S**ingle **P**recision files (SPx)
    - No keyword association.
    - Enables SPx tab
    - Backwards compatibility: Enabled if any SPx time values are specified
- Enable NetCDF output files
    - Not available when SPx output is enabled
    - No keyword association.
    - Enables NetCDF tab



SPx (tab)

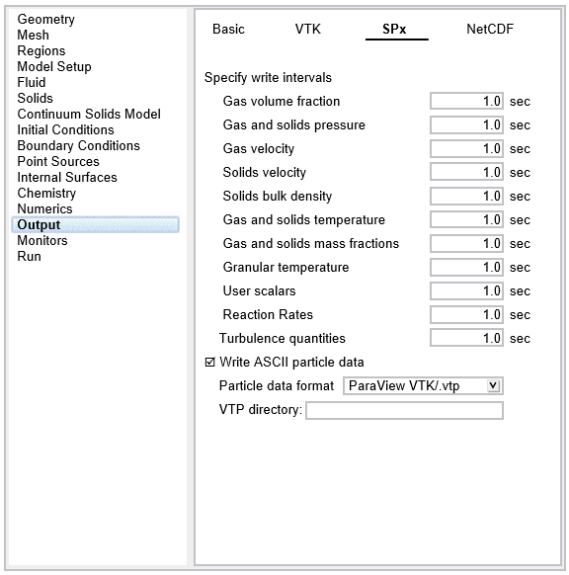
Note: Technically, MFIX will now permit a user to mix-and-match the SPx output files meaning that some can be written and others not. However, this is likely to break the ParaView reader. Therefore, if the "Write binary SPx" checkbox is enabled, output is required for all SPx files. Otherwise, all should remain unspecified to skip writing the SPx files.

- Write interval for gas volume fraction
    - Sets keyword SPX_DT(1)
    - DEFAULT value of 1.0
    - Required if SPx data is enabled.
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids pressure
    - Sets keyword SPX_DT(2)
    - Required if SPx data is enabled.
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas velocity
    - Sets keyword SPX_DT(3)
    - Required if SPx data is enabled.
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT

- Write interval for solids velocity
    - Required if SPx data is enabled.
    - Sets keyword SPX_DT(4)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for solids bulk density
    - Sets keyword SPX_DT(5)
    - Required if SPx data is enabled.
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids temperature
    - Sets keyword SPX_DT(6)
    - Required if SPx data is enabled and solving any energy equations.
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids mass fractions
    - Sets keyword SPX_DT(7)
    - Required if SPx data is enabled and solving any species equations.
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for granular temperature
    - Sets keyword SPX_DT(8)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for user defined scalars
    - Sets keyword SPX_DT(9)
    - Required if SPx data is enabled and solving any user defined scalar equations
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for reaction rates
    - Sets keyword SPX_DT(10)
    - Required if SPx data is enabled and NRR > 0 (see below)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Number of reaction rates to write
    - Specification always available
    - Sets keyword NRR
    - DEFAULT value of 0
    - Error check: value must be greater than or equal to 0
- Write interval for turbulence quantities
    - Sets keyword SPX_DT(11)
    - Required if SPx data is enabled and TURBULENCE_MODEL = “K_EPSILON”
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT

- Write ASCII particle data
    - Selection only available if DEM or PIC solids
    - Sets keyword PRINT_DES_DATA
    - DEFAULT value of .TRUE.
- Specify VTP Directory
    - Specification only if PRINT_DES_DATA = .TRUE.
    - Sets keyword VTP_DIR
    - No default (empty string)
- Select particle data format

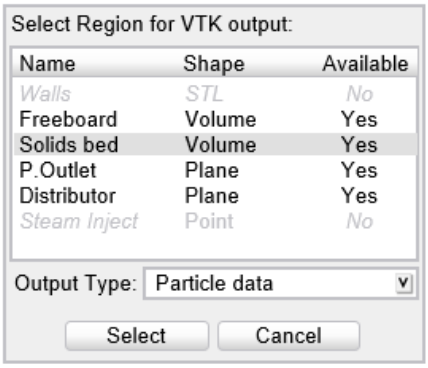
- Selection only available if DEM or PIC solids and PRINT_DES_DATA = .TRUE.
- Sets keyword DES_OUTPUT_TYPE
- Available Selections
  - *ParaView - VTK/.vtp* [DEFAULT]
  - *Tecplot - .dat*



VTK (tab)

Icons and table similar to IC/BC/PS/IS for adding VTK regions. This section requires WRITE_VTK_FILES = .TRUE.

- 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 a VTK region.
  - Users cannot select inapplicable regions.
  - VTK regions can be points, planes, or volumes (not STLs)
  - Regions can define multiple VTK regions.
- Select Output type
  - Selection is required
  - Available selections:
    - *Cell data*
      - Selection always available
      - Set keyword VTK_DATA(#) to 'C'
    - *Particle data*
      - Selection only available with DEM or PIC solids
      - Sets keyword VTK_DATA(#) to 'P'



Cell data sub-pane

There is a need for some hand waving here. Many mfix.dat files may use a different specification for VTK input. There will need to be a way of catching the 'old' format and converting it to this input style.

- Specify filename base
  - Specification is required.
  - Sets keyword VTK_FILEBASE(#)
  - DEFAULT value of region name
- Specify write interval
  - Specification is required
  - Sets keyword VTK_DT(#)
  - DEFAULT value of 1.0 (must write)
- Specify region x-axis slices
  - Specification always available
  - Sets keyword VTK_NXS(#)
  - DEFAULT value of 0
- Specify region y-axis slices
  - Specification always available
  - Sets keyword VTK_NYS(#)
  - DEFAULT value of 0
- Specify region z-axis slices
  - Specification always available
  - Sets keyword VTK_NZS(#)
  - DEFAULT value of 0

Fluid Phase (tab?)

- Enable writing gas volume fraction
  - Selection always available
  - Sets keyword VTK_EP_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas pressure
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_P_G(#)

  - DEFAULT value .FALSE.
- Enable writing solids pressure
  - Requires TFM solids
  - Sets keyword VTK_P_STAR
  - DEFAULT value .FALSE.
- Enable writing gas velocity vector
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_VEL_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas velocity x-component
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_U_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas velocity y-component
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_V_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas velocity z-component
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_W_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas temperature
  - Requires fluid solver (RO_G0 /= 0.0) and ENERGY_EQ = .TRUE.
  - Sets keyword VTK_T_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas species N (**an entry for each defined species**)
  - Requires defined gas phase species
  - Sets keyword VTK_X_G(#,N)
  - DEFAULT value .FALSE.
- Enable writing gas temperature
  - Requires fluid solver (RO_G0 /= 0.0) and ENERGY_EQ = .TRUE.
  - Sets keyword VTK_T_G(#)
  - DEFAULT value .FALSE.
- Enable writing gas species N
  - Requires fluid solver (RO_G0 /= 0.0) and SPECIES_EQ(0) = .TRUE.
  - Sets keyword VTK_X_G(#,N)
  - DEFAULT value .FALSE.
- Enable writing turbulent kinetic energy
  - Requires fluid solver (RO_G0 /= 0.0) and TURBULENCE_MODEL='K_EPSILON'
  - Sets keyword VTK_K_TURB_G(#)
  - DEFAULT value of .FALSE.
- Enable writing turbulent dissipation
  - Requires fluid solver (RO_G0 /= 0.0) and TURBULENCE_MODEL='K_EPSILON'
  - Sets keyword VTK_E_TURB_G(#)
  - DEFAULT value of .FALSE.

- Enable writing reaction rates
  - Requires nRR > 0
  - Sets keyword VTK_RRATE(#)
  - DEFAULT value .FALSE.

Solids Phase (tab?)

- Enable writing solids velocity vector
  - Requires TMF solids
  - Sets keyword VTK_VEL_S(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids velocity x-component
  - Requires TMF solids
  - Sets keyword VTK_U_S(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids velocity y-component
  - Requires TMF solids
  - Sets keyword VTK_V_S(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids velocity z-component
  - Requires TMF solids
  - Sets keyword VTK_W_S(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids bulk density
  - Requires TMF solids
  - Sets keyword VTK_ROP_S(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids temperature
  - Requires TFM solids and ENERGY_EQ = .TRUE.
  - Sets keyword VTK_S_G(#,#)
  - DEFAULT value .FALSE.
- Enable writing solids phase M, species N
  - Requires TFM solids and SPECIES_EQ(#) = .TRUE.
  - Sets keyword VTK_X_S(#,M,N)
  - DEFAULT value .FALSE.
- Enable writing solids phase granular temperature
  - Requires TFM solids and KT_TYPE /= “ALGEBRAIC”
  - Sets keyword VTK_THETA_M(#,#)
  - DEFAULT value .FALSE.

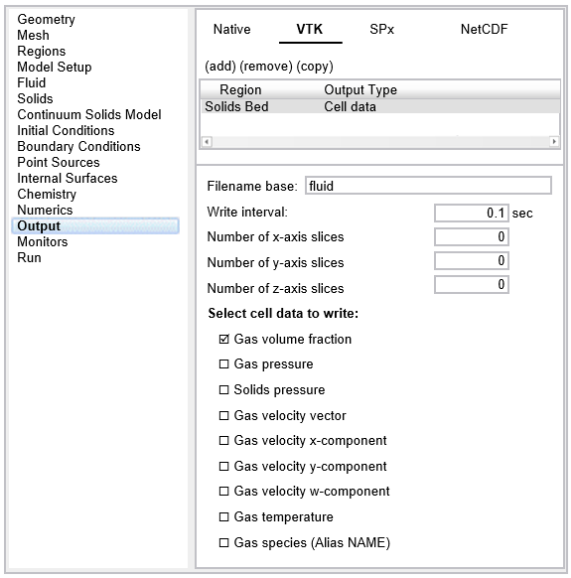
Scalar (tab?)

- Enable writing user defined scalar
  - Requires NSCALAR > 0
  - Sets keyword VTK_SCALAR(#)
  - DEFAULT value .FALSE.

Other (tab?)

- Enable writing vorticity
  - Requires fluid solver (RO_G0 /= 0.0)
  - Sets keyword VTK_VORTICITY (#)
  - Sets keyword VTK_LAMBDA_2(#)
  - DEFAULT value .FALSE.
- Enable writing partition
  - Sets keyword VTK_PARTITION(#)
  - DEFAULT value .FALSE.
- Enable writing boundary ID
  - Sets keyword VTK_BC_ID(#)
  - DEFAULT value .FALSE.

- Enable writing wall distance
  - Sets keyword VTK_DWALL(#)
  - DEFAULT value .FALSE.
- Enable writing cell index
  - Sets keyword VTK_IJK(#)
  - DEFAULT value .FALSE.
-



Particle data sub-pane

There is a need for some hand waving here. Many mfix.dat files may use a different specification for VTK input. There will need to be a way of catching the 'old' format and converting it to this input style.

- Specify filename base
  - Specification is required.
  - Sets keyword VTK_FILEBASE(#)
  - DEFAULT value of region name
- Specify write interval
  - Specification is required
  - Sets keyword VTK_DT(#)
  - DEFAULT value of 1.0 (must write)
- Specify region x-axis slices
  - Specification always available
  - Sets keyword VTK_NXS(#)
  - DEFAULT value of 0
- Specify region y-axis slices
  - Specification always available
  - Sets keyword VTK_NYS(#)
  - DEFAULT value of 0
- Specify region z-axis slices

  - Specification always available
  - Sets keyword VTK_NZS(#)
  - DEFAULT value of 0

- Enable writing particle diameter
  - Requires DEM or PIC solids
  - Sets keyword VTK_PART_DIAMETER(#)
  - DEFAULT value .FALSE.
- Enable writing particle translational velocity
  - Requires DEM or PIC solids
  - Sets keyword VTK_PART_VEL(#)
  - DEFAULT value .FALSE.
- Enable writing particle rotational velocity
  - Requires DEM or PIC solids
  - Sets keyword VTK_ANGULAR_VEL(#)
  - DEFAULT value .FALSE.
- Enable writing particle orientation
  - Requires DEM or PIC solids
  - Sets keyword PARTICLE_ORIENTATION = .TRUE.
  - Sets keyword VTK_ORIENTATION(#)
  - DEFAULT value .FALSE.
- Enable writing particle user variable
  - Requires DEM or PIC solids and DES_USR_VAR > 0
  - Sets keyword VTK_PART_USR_VAR(#,#)
  - DEFAULT value .FALSE.
- Enable writing particle rotational velocity
  - Requires DEM or PIC solids
  - Sets keyword VTK_ANGULAR_VEL(#)
  - DEFAULT value .FALSE.
- Enable writing particle temperature
  - Requires DEM or PIC solids and ENERGY_EQ=.TRUE.
  - Sets keyword VTK_PART_TEMP(#)
  - DEFAULT value .FALSE.
- Enable writing particle species composition
  - Requires DEM or PIC solids and any SPECIES_EQ=.TRUE.
  - Sets keyword VTK_PART_X_S(#)
  - DEFAULT value .FALSE.
- Enable writing particle MPI rank
  - Requires DEM or PIC solids
  - Sets keyword VTK_PART_RANK(#)
  - DEFAULT value .FALSE.
- Enable writing particle global ID
  - Requires DEM or PIC solids
  - Sets keyword VTK_PART_ID(#)
  - DEFAULT value .FALSE.

NetCDF (tab)

Note: NetCDF support 'piggy-backs' off of the SPx keywords. The output time values are specified via SPX_DT while NetCDF output is triggered by a BWRITE_NETCDF flag. To make this less opaque to users, both SPx and netCDF output cannot be enabled at the same time.

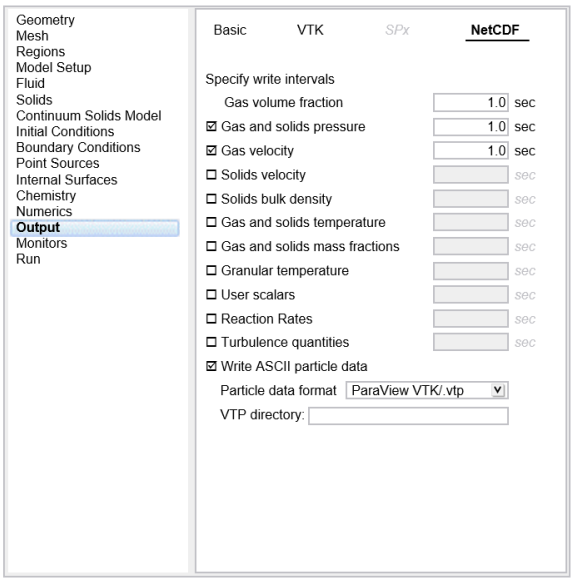
- Write interval for gas volume fraction

    - Sets keyword BWRITE_NETCDF(1) = .TRUE.
    - Sets keyword SPX_DT(1)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids pressure
    - Sets keyword BWRITE_NETCDF(2) = .TRUE.
    - Sets keyword BWRITE_NETCDF(3) = .TRUE.
    - Sets keyword SPX_DT(2)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas velocity
    - Sets keyword BWRITE_NETCDF(4) = .TRUE.
    - Sets keyword SPX_DT(3)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for solids velocity
    - Sets keyword BWRITE_NETCDF(5) = .TRUE.
    - Sets keyword SPX_DT(4)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for solids bulk density
    - Sets keyword BWRITE_NETCDF(6) = .TRUE.
    - Sets keyword SPX_DT(5)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids temperature
    - Only available when solving energy equations
    - Sets keyword BWRITE_NETCDF(7) = .TRUE.
    - Sets keyword BWRITE_NETCDF(8) = .TRUE.
    - Sets keyword SPX_DT(6)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for gas and solids mass fractions
    - Only available when solving species equations
    - Sets keyword BWRITE_NETCDF(9) = .TRUE.
    - Sets keyword BWRITE_NETCDF(10) = .TRUE.
    - Sets keyword SPX_DT(7)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for granular temperature
    - Only available when KT_TYPE =/ 'ALGEBRAIC'
    - Sets keyword BWRITE_NETCDF(11) = .TRUE.
    - Sets keyword SPX_DT(8)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for user defined scalars
    - Only available when solving any user defined scalar equations
    - Sets keyword BWRITE_NETCDF(12) = .TRUE.
    - Sets keyword SPX_DT(9)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Write interval for reaction rates
    - Only available if NRR > 0 (see below)
    - Sets keyword BWRITE_NETCDF(13) = .TRUE.

    - Sets keyword SPX_DT(10)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT
- Number of reaction rates to write
    - Specification always available
    - Sets keyword NRR
    - DEFAULT value of 0
    - Error check: value must be greater than or equal to 0
- Write interval for turbulence quantities
    - Only available if TURBULENCE_MODEL = "K_EPSILON"
    - Sets keyword BWRITE_NETCDF(14) = .TRUE.
    - Sets keyword SPX_DT(11)
    - DEFAULT value of 1.0
    - Error check: value must be greater than or equal to RES_DT

This is the same particle section as the SPx section.

- Write ASCII particle data
    - Selection only available if DEM or PIC solids
    - Sets keyword PRINT_DES_DATA
    - DEFAULT value of .TRUE.
- Specify VTP Directory
    - Specification only if PRINT_DES_DATA = .TRUE.
    - Sets keyword VTP_DIR
    - No default (empty string)
- Select particle data format
    - Selection only available if DEM or PIC solids and PRINT_DES_DATA = .TRUE.

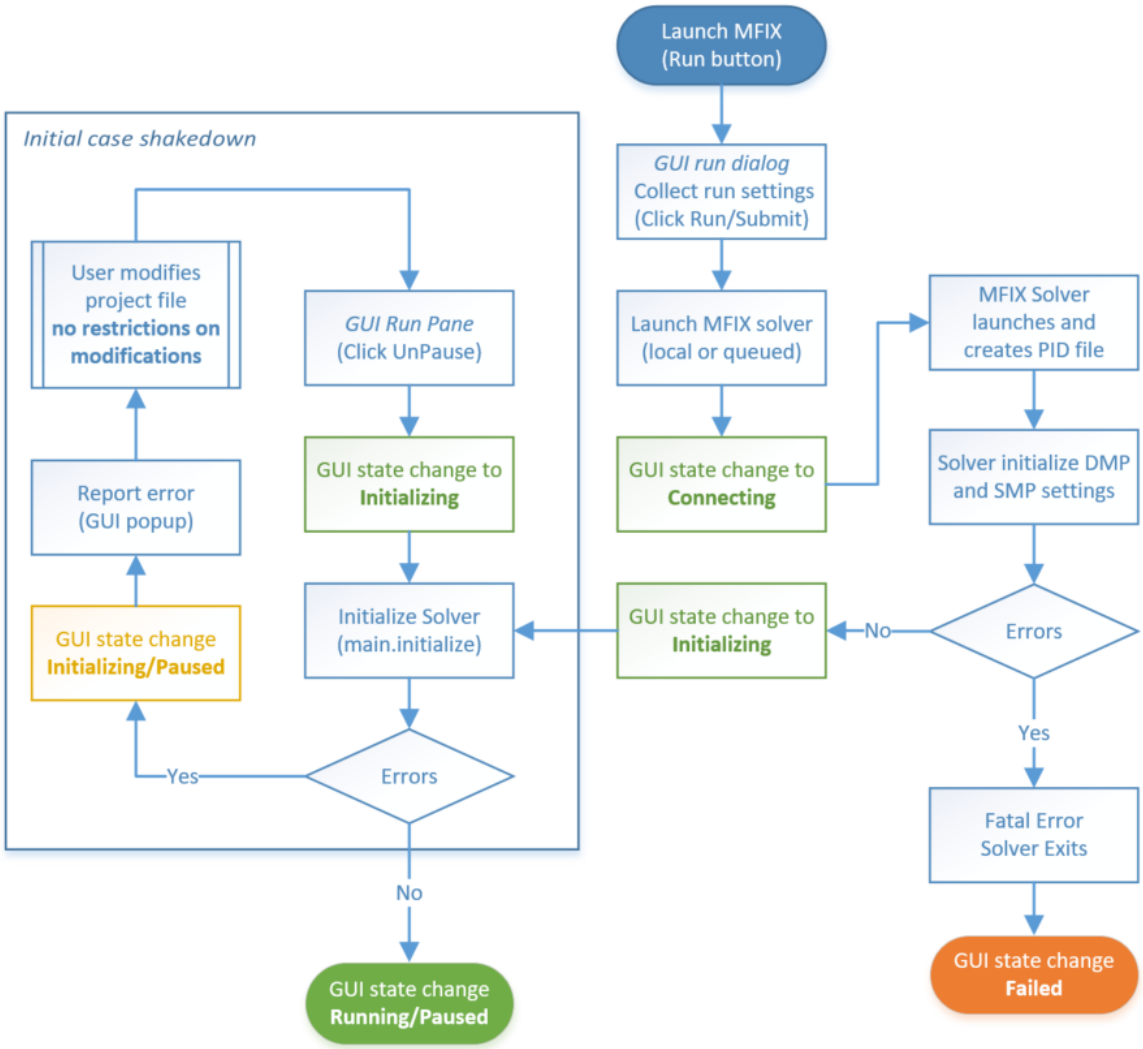


3.1.3 Job submission/Interactive Control

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) Processes the case file (*.mfx)
4) Check validity of project settings
    a. Check and setup base background mesh
    b. Setup MPI domain decomposition
    c. Preform sanity checks on user inputs
    d. Set flags and loop structures for background mesh
    e. Invoke Cartesian grid cut-cell preprocessing
    f. Allocate data arrays
5) Process RES (restart) files
    a. Save current state for new runs
    b. Read RES files for restarts
6) Setup initial field states prior to time march



yeStep 4 is where the majority of failures will be caught when starting the MFIX solver. The solver should catch the error and report it back to the GUI so the user may correct the issue. To facilitate

3.1.4 Workflow Mode

Workflow mode utilizes pyqtnode's graphical programing 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.

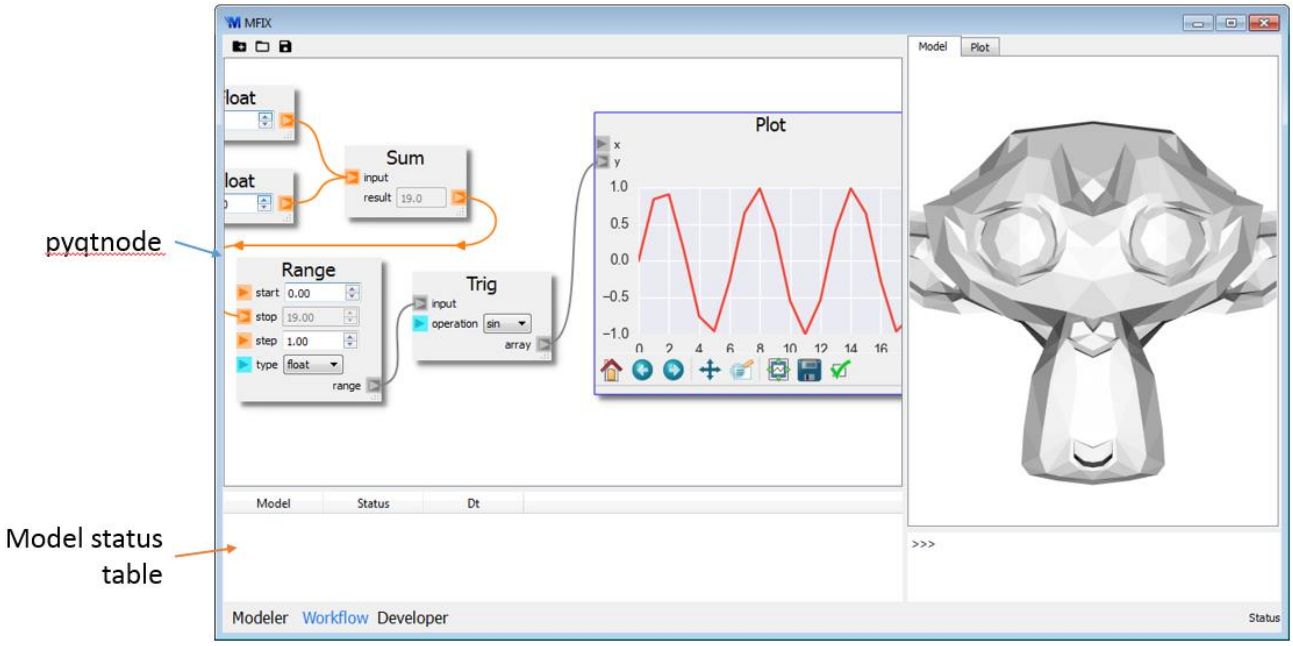
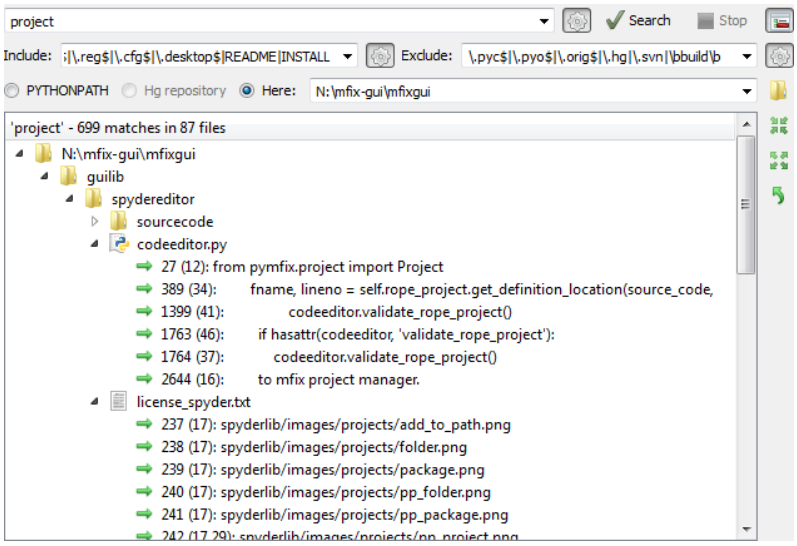


Figure 3: General layout of the "Workflow" mode.

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 were 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 (ubunutu, 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 s 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.>

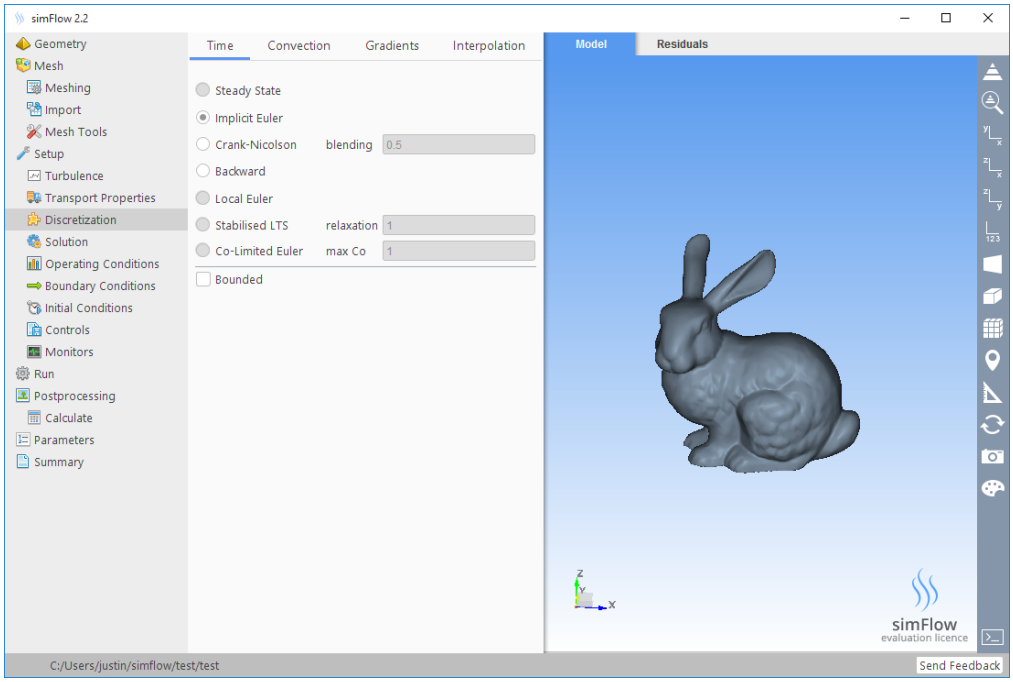
Appendix C: To Be Determined List

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

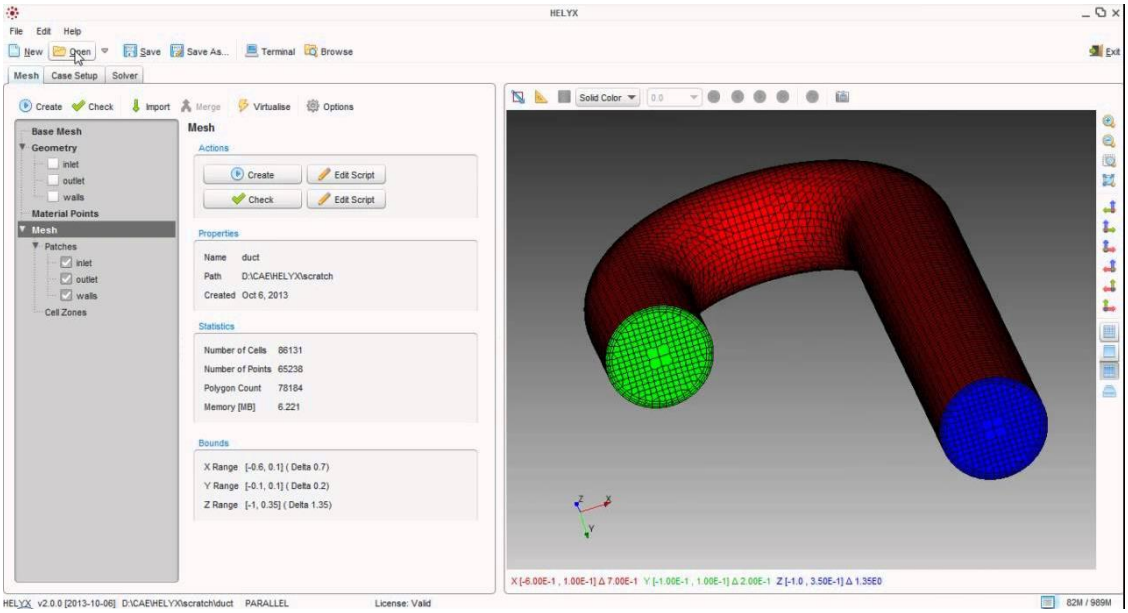
Appendix D: UI Resources

6.1.1 Other CFD UI's

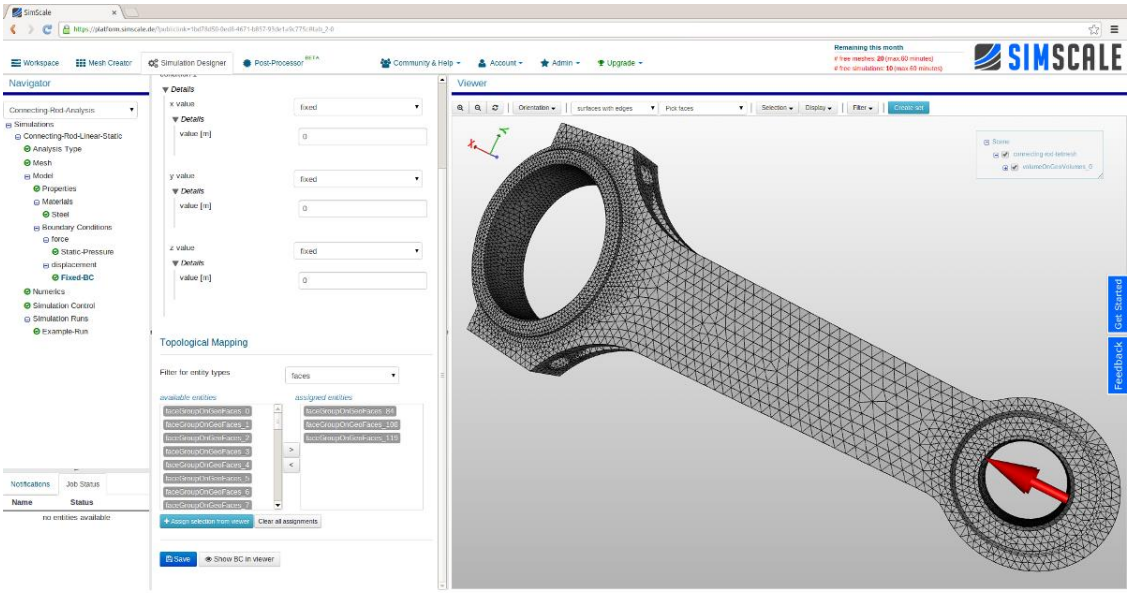
SimFlow



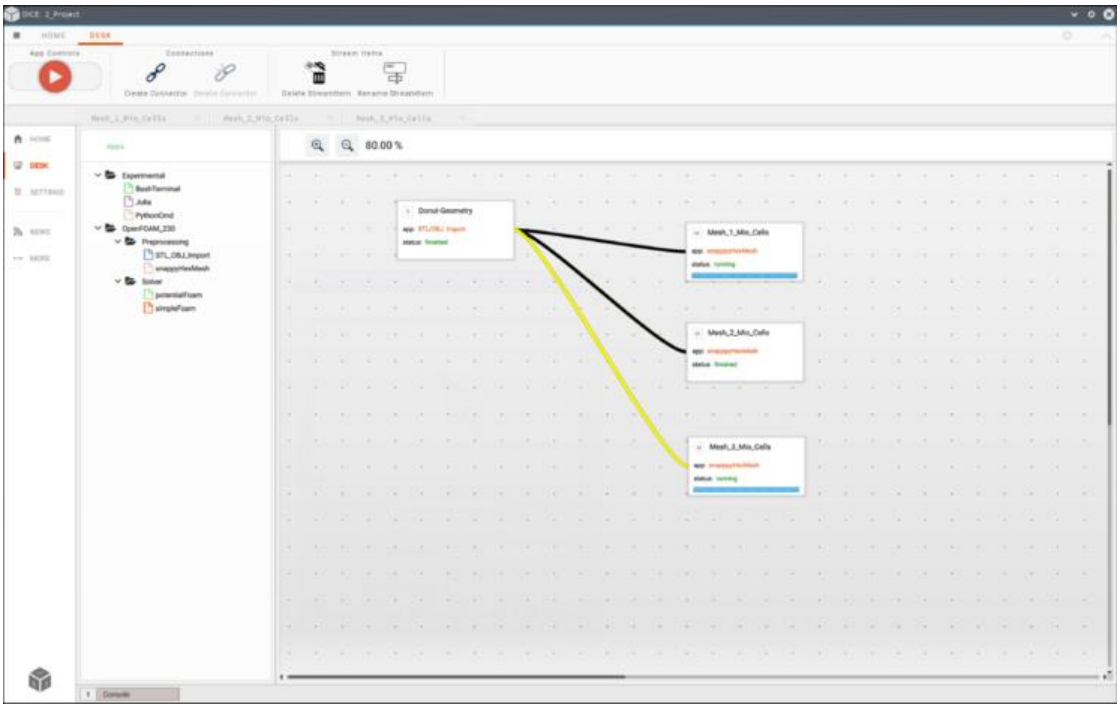
HELYX-OS



SimScale



DICEhub



Appendix E: Calculating Variable Solids Density

Calculating the solids density is done in the context an initial condition (IC) region, but it is the same calculations hold for boundary conditions (BCs).

1) Calculate the baseline density, RO_S0(M) = $1.0/\text{sum}_k$(X_S0(M,K)/RO_XS0(M,K))
2) Calculate the solids density:
    a. Let I=INERT_SPECIES(M)
    b. IC_RO_S(M) = RO_S0(M) * X_S0(M,I)/IC_X_S(#,M,I)

Note that RO_S0 is used for example and that it should not be set in the input deck file for variable solid density cases.