Silane Deposition: Setup and Analysis

CPFD Software

www.cpfd-software.com

Silane Deposition

System Pressure: 1.358 bar

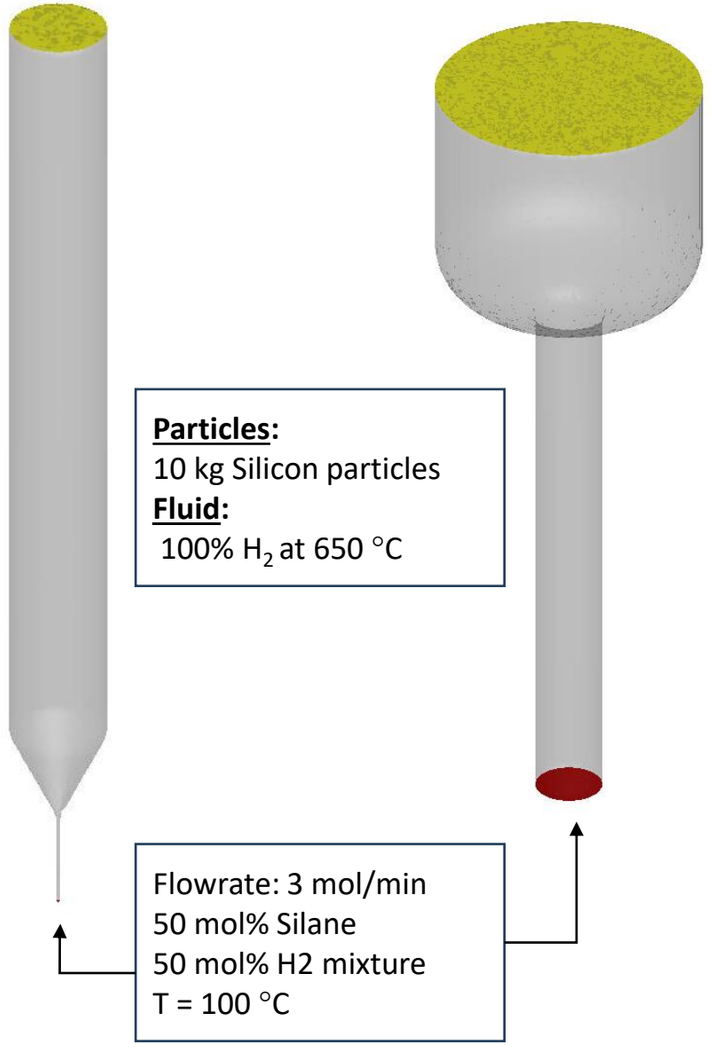
Model of fluidized bed system with two different geometries based on Parker (2011)

Case 1: Screen Mesh

Case 2: Nozzle

The only difference in the simulations will be the boundary conditions:

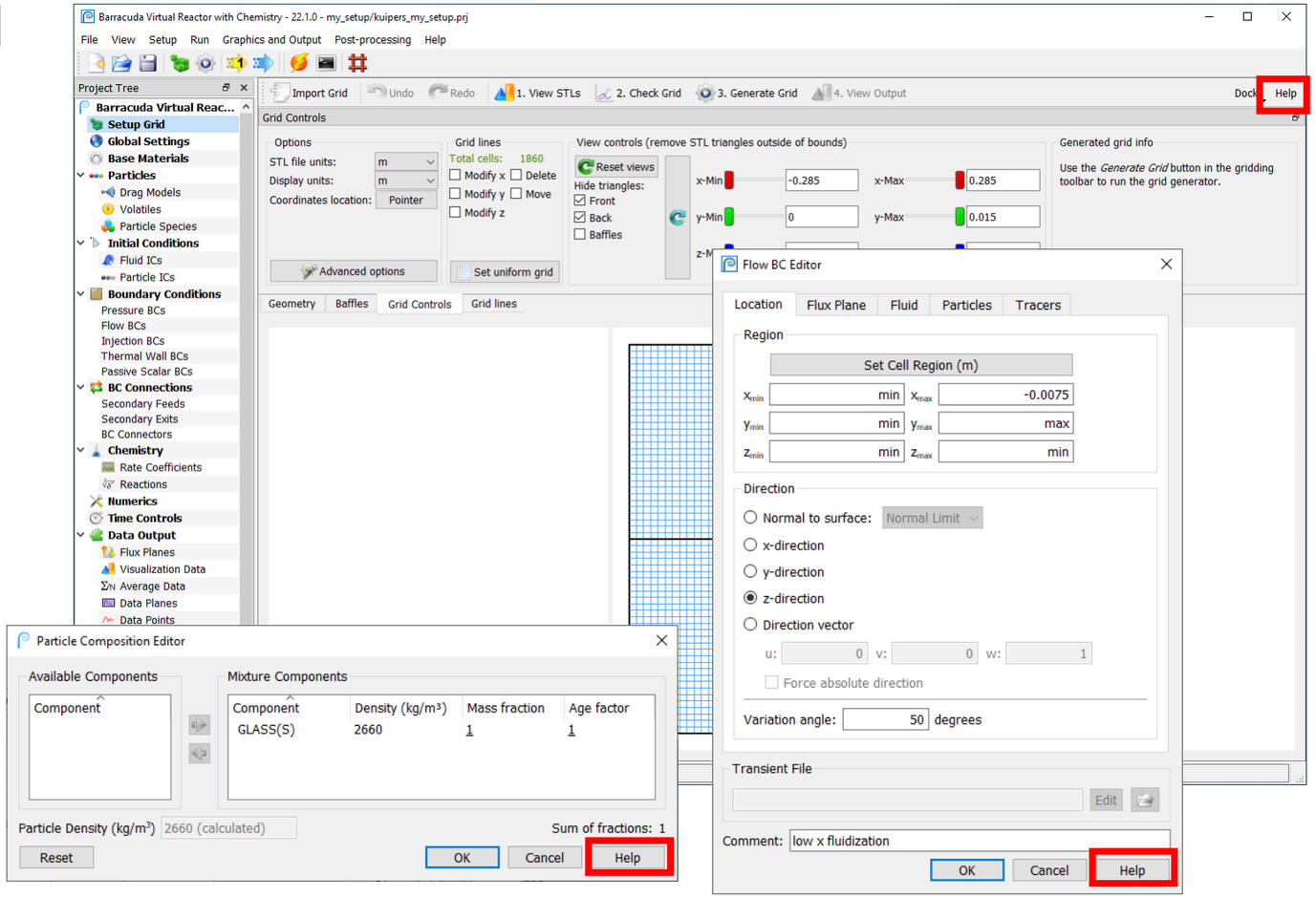
Note: Unless otherwise specified in the title, the following model setup instructions apply for both geometries



How to Get More Information

All training materials have a limited amount of information about Barracuda and the GUI.

If you want to learn more, click on the Help button in the relevant dialog. This brings up the corresponding section of the User Manual.



Project File

We will demonstrate how to run the project with the case of 57% mole fraction feed to SiH4 for each reactor geometry. Download the my-setup folder and locate the following directories

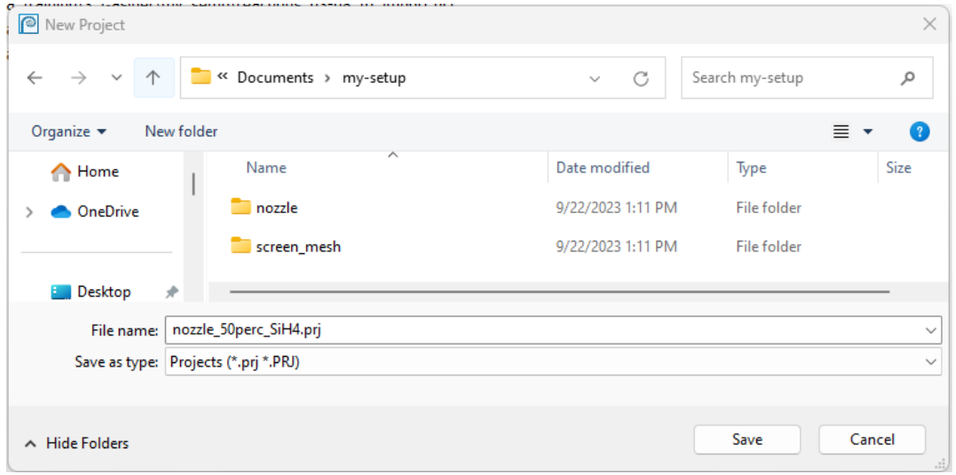
my-setup\nozzle\57perc_SiH4

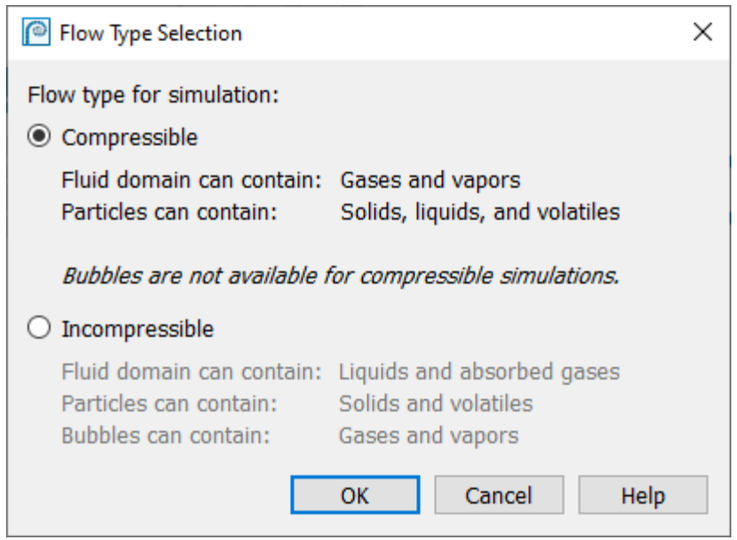
my-setup\screen_mesh\57perc_SiH4

Create projects in the appropriate directories with the following names

nozzle_57percSiH4.prj

screen_mesh_57percSiH4.prj





Screen Mesh: Setup Grid

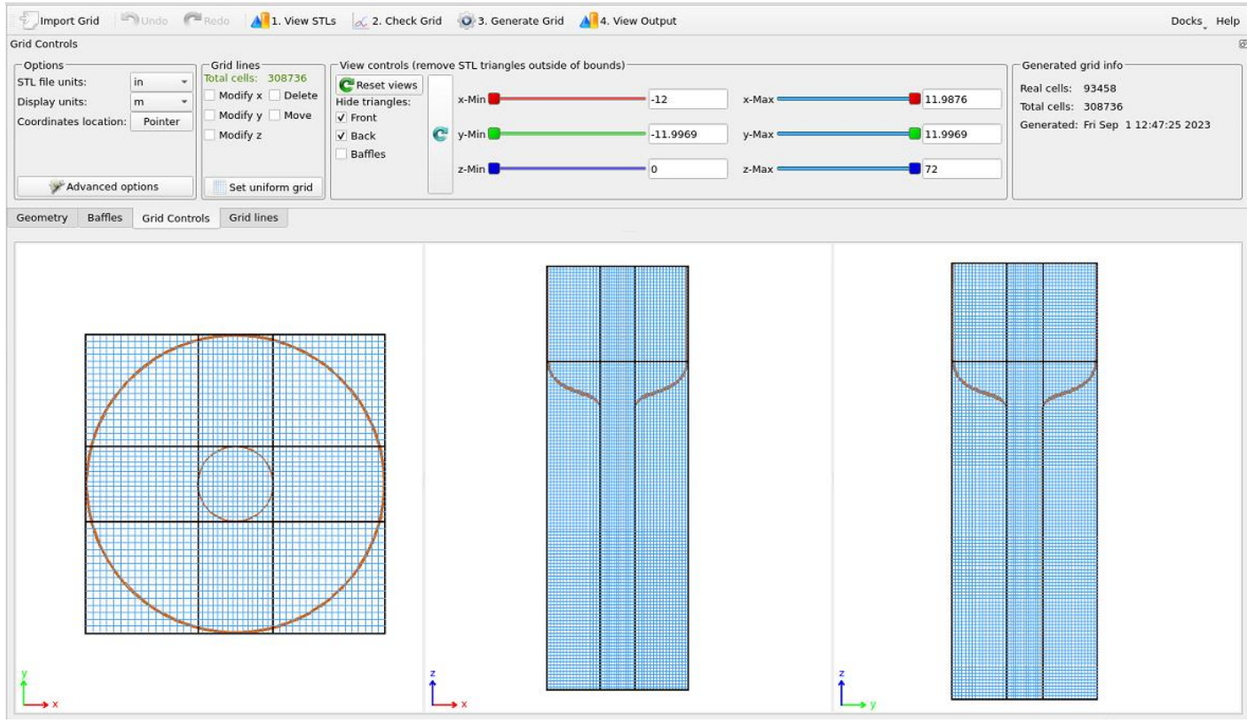
In the **screen_mesh/screen_mesh_57perc_SiH4.prj** file

Geometry tab:

- Add 2010-07-02_silane_reactor_flat_inlet.stl

Controls tab:

- Set STL file units to inches



Nozzle: Setup Grid

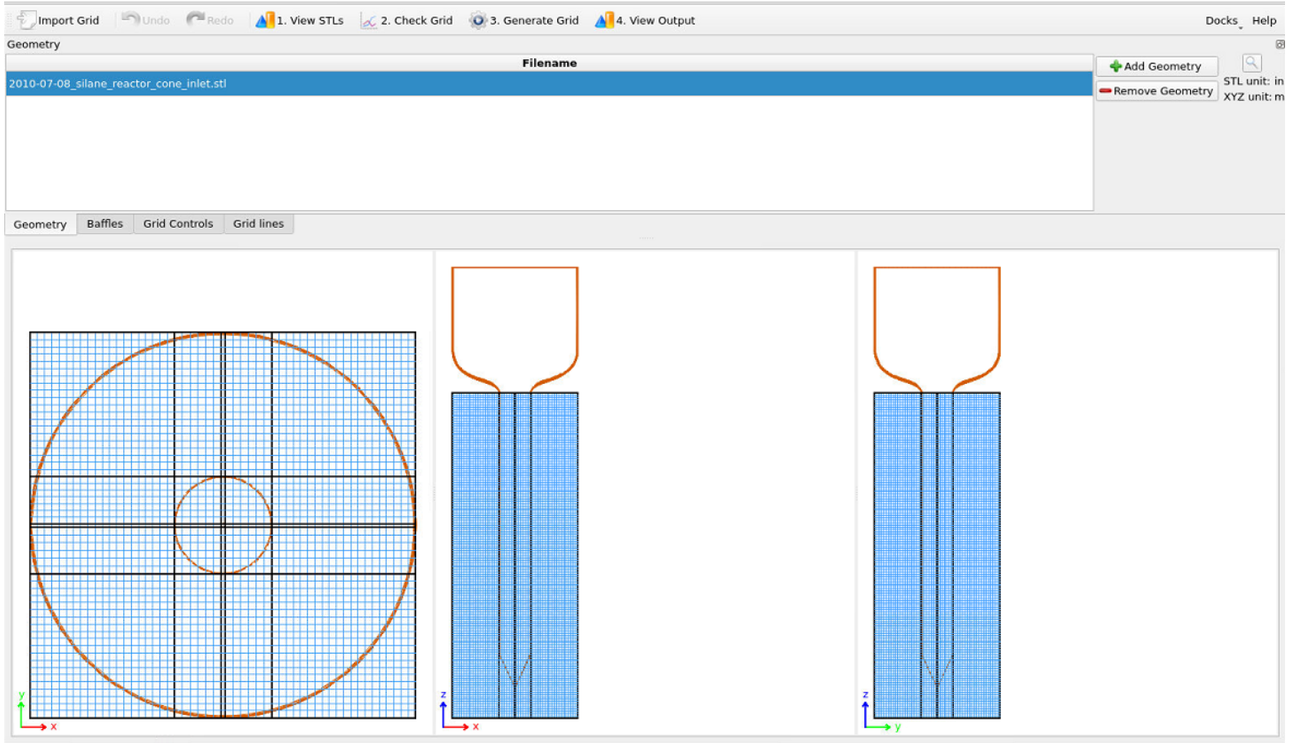
In the **nozzle/nozzle_57perc_SiH4.prj** file

Geometry tab:

- Add 2010-07-02_silane_reactor_cone.stl

Controls tab:

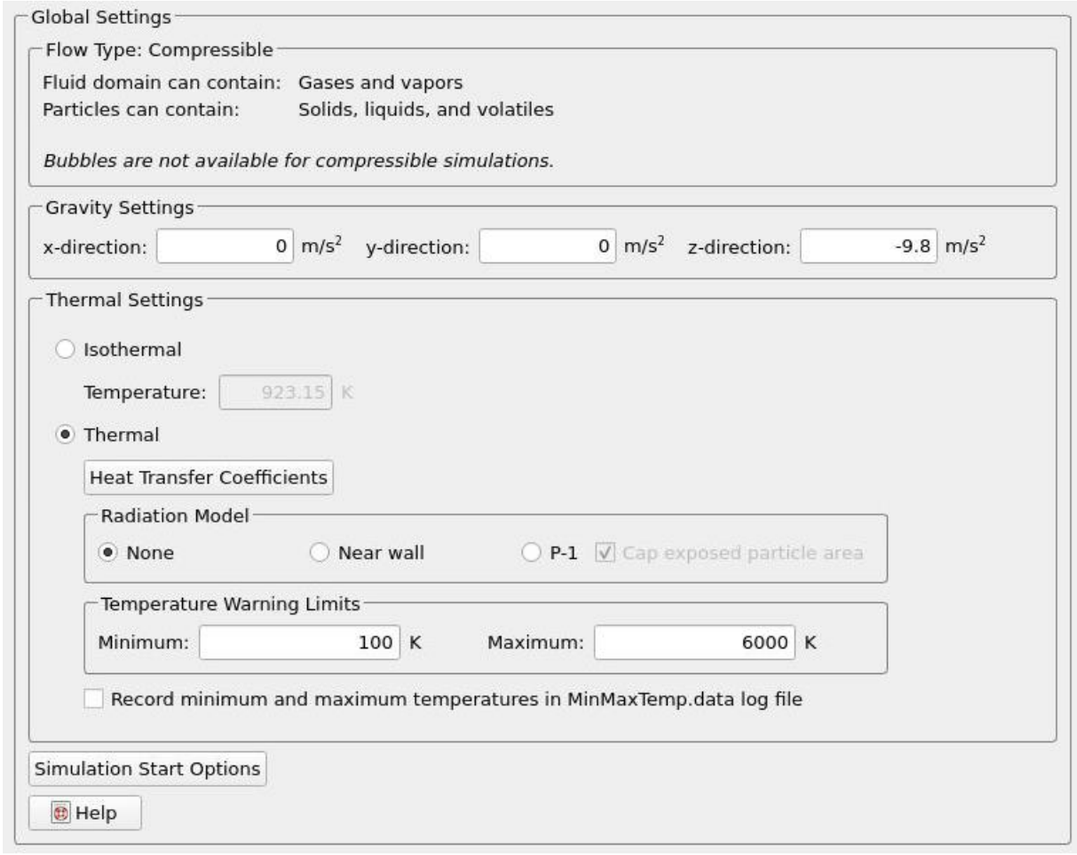
- Set STL file units to inches



Global Settings

Set Gravity in the z-direction

Select Thermal to enable thermal calculations with None selected for radiation model

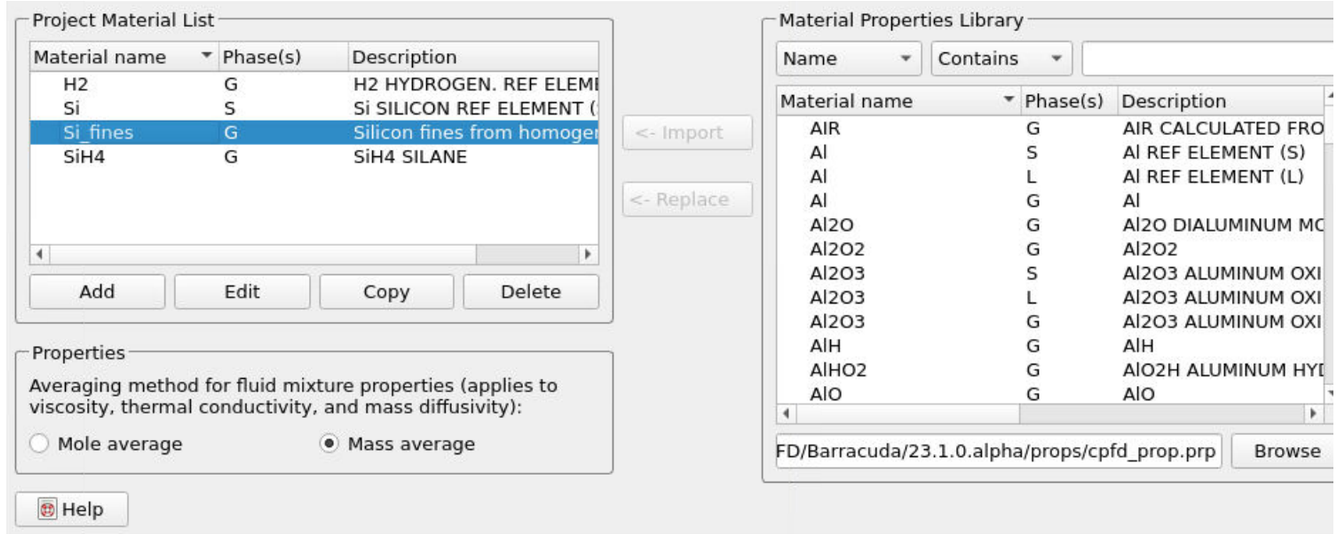


Base Materials

Import H2, Si(S), and SiH4

Add Si_fines (Silicon fines)

- Phase: Gas
  - Note that gas is chosen here due to the reaction chemistry. Barracuda does not have the functionality for deposition without a seed particle (as is done in the homogeneous reaction)
- MW = 28 g/mol
- Viscosity = 3e-5 Pa*s

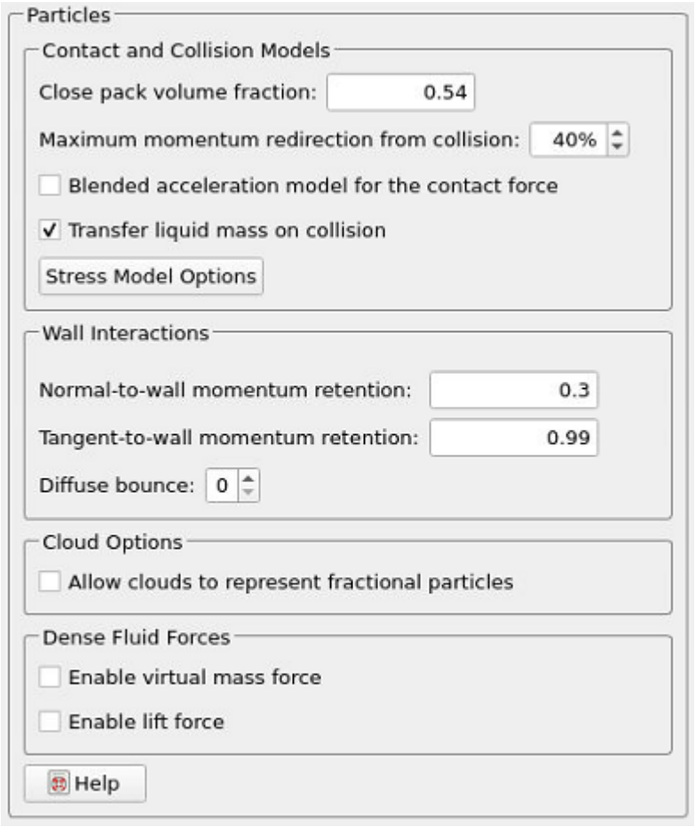


Particles

Set Close pack volume fraction: 0.54

Normal-to-wall momentum retention: 0.3

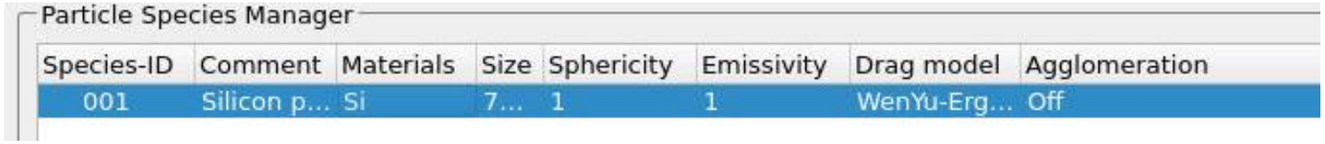
Tangent-to-wall momentum retention: 0.99



Particles Species

Create a Silicon particle species with the following properties:

- 100% Silicon(S)
- Size range: 75 – 425 micron-diameter
- WenYu-Ergun drag model



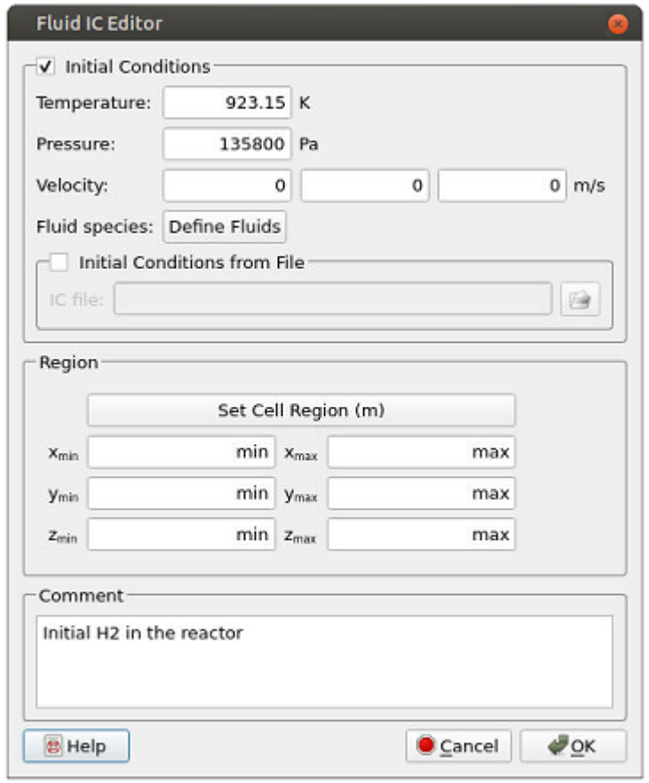
Screen Mesh: Fluid and Particle ICs

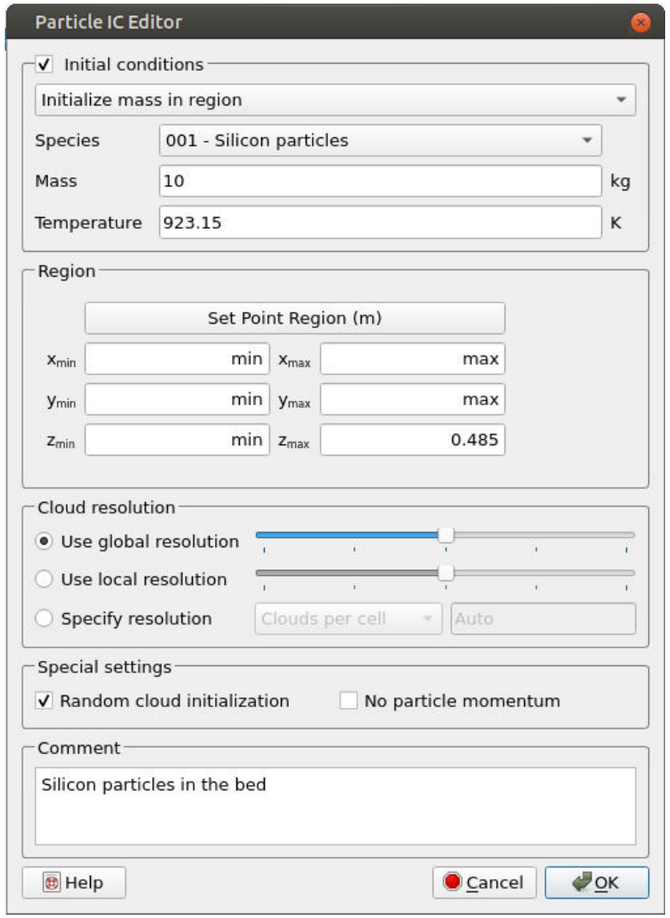
Fluid IC

- Pressure = 135800 Pa
- Fluid species = 100% H2

Particle IC

- Initialize mass in region
- Species = Silicon (S)
- Mass = 10 kg
- Set region to min, max for x and y, z-min to min, z-max to 0.485





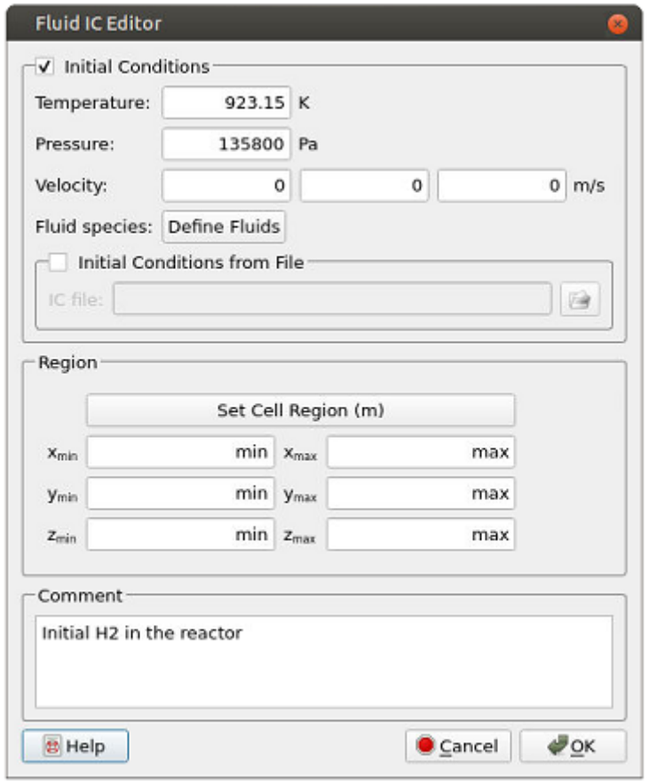
Nozzle: Fluid and Particle ICs

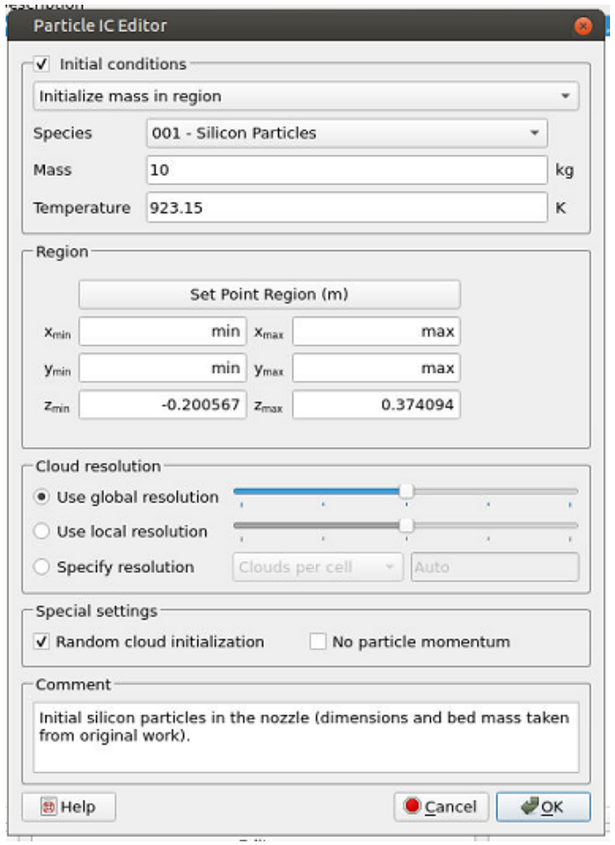
Fluid IC

- Pressure = 135800 Pa
- Fluid species = 100% H2

Particle IC

- Initialize mass in region
- Species = Silicon (S)
- Mass = 10 kg
- Set region to min, max for x and y, z-min to -0.2, and z-max to 0.4





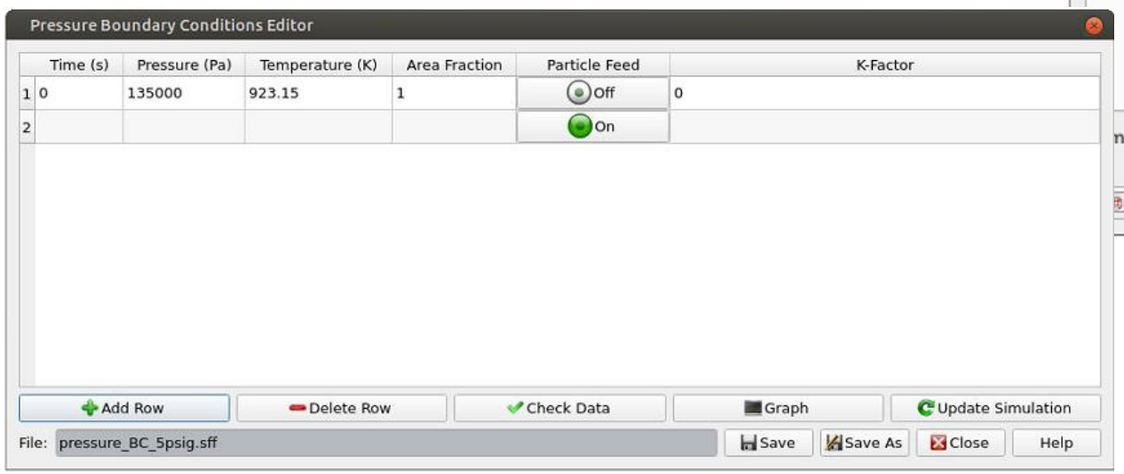
Pressure BC

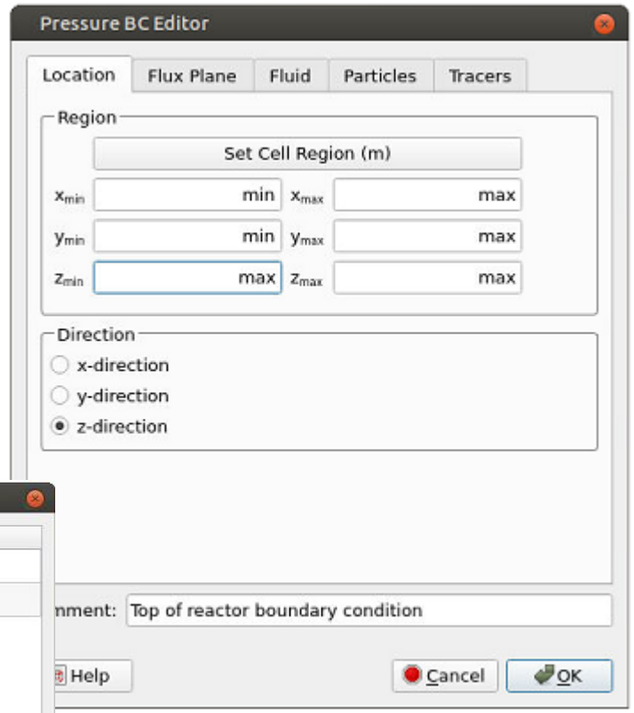
Add a pressure BC for the reactor top with the following region defined

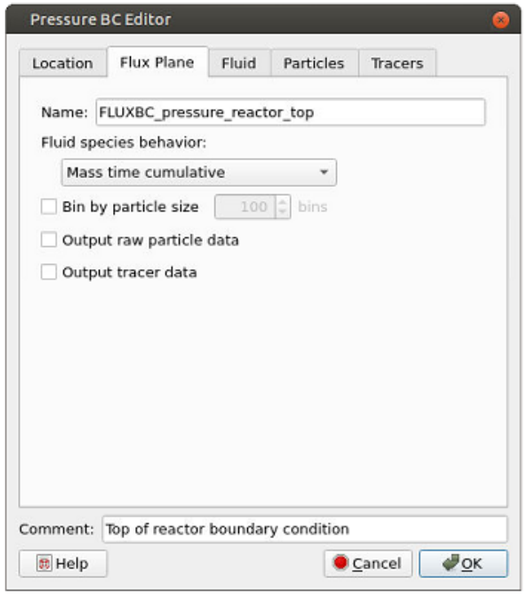
In the fluid pane, select 100% H2

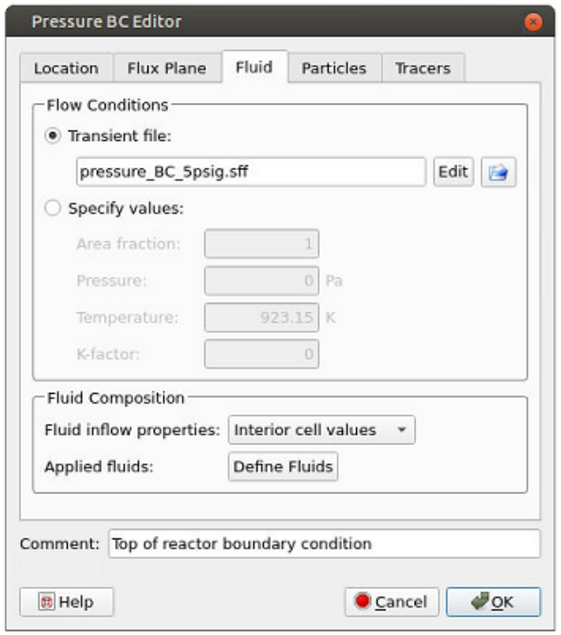
In the flux plane tab, ensure that *Mass Fraction* is selected

Define external pressure of 135000 Pa and temperature of 923.15 K through an sff file:





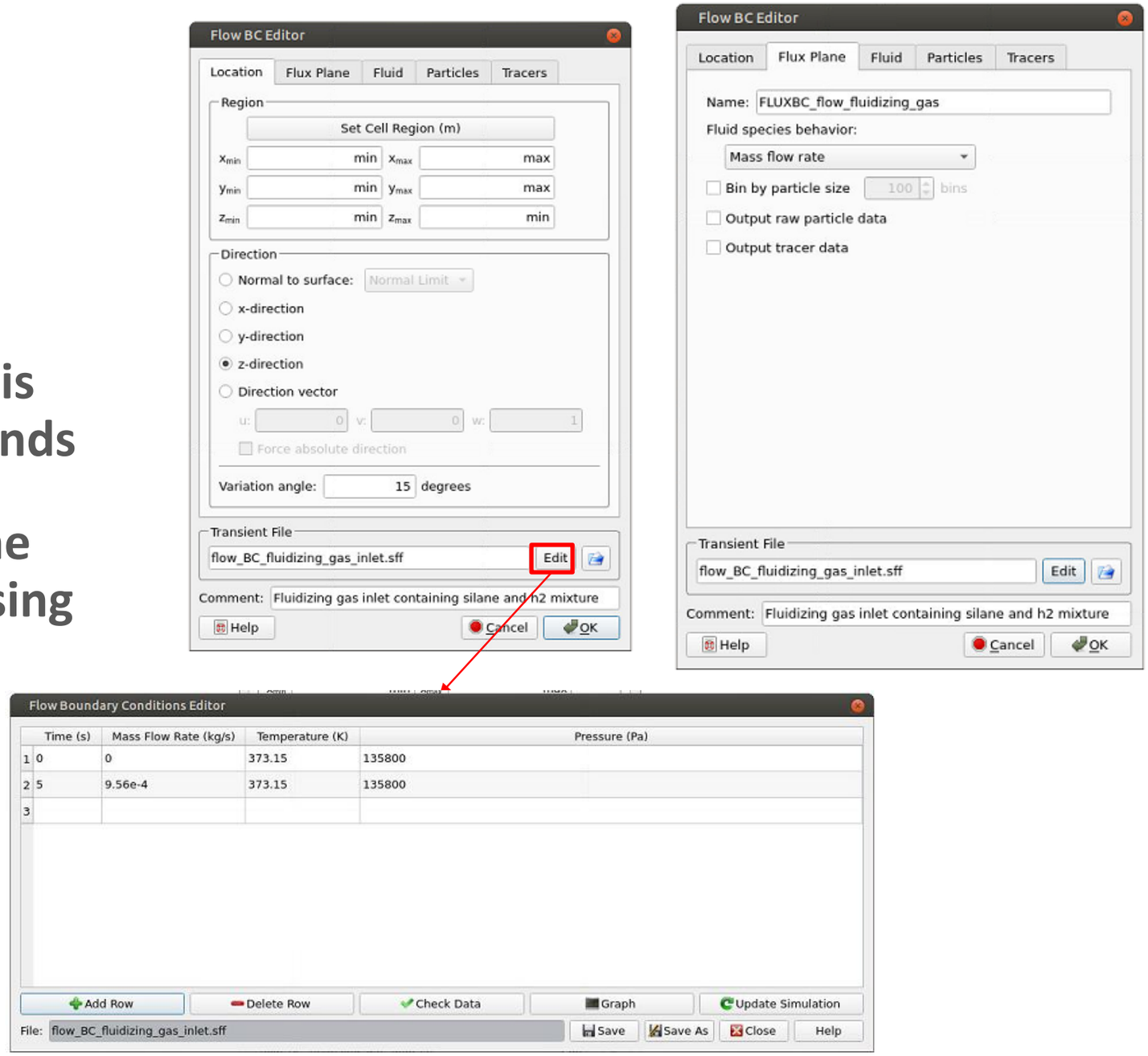




Flow BC

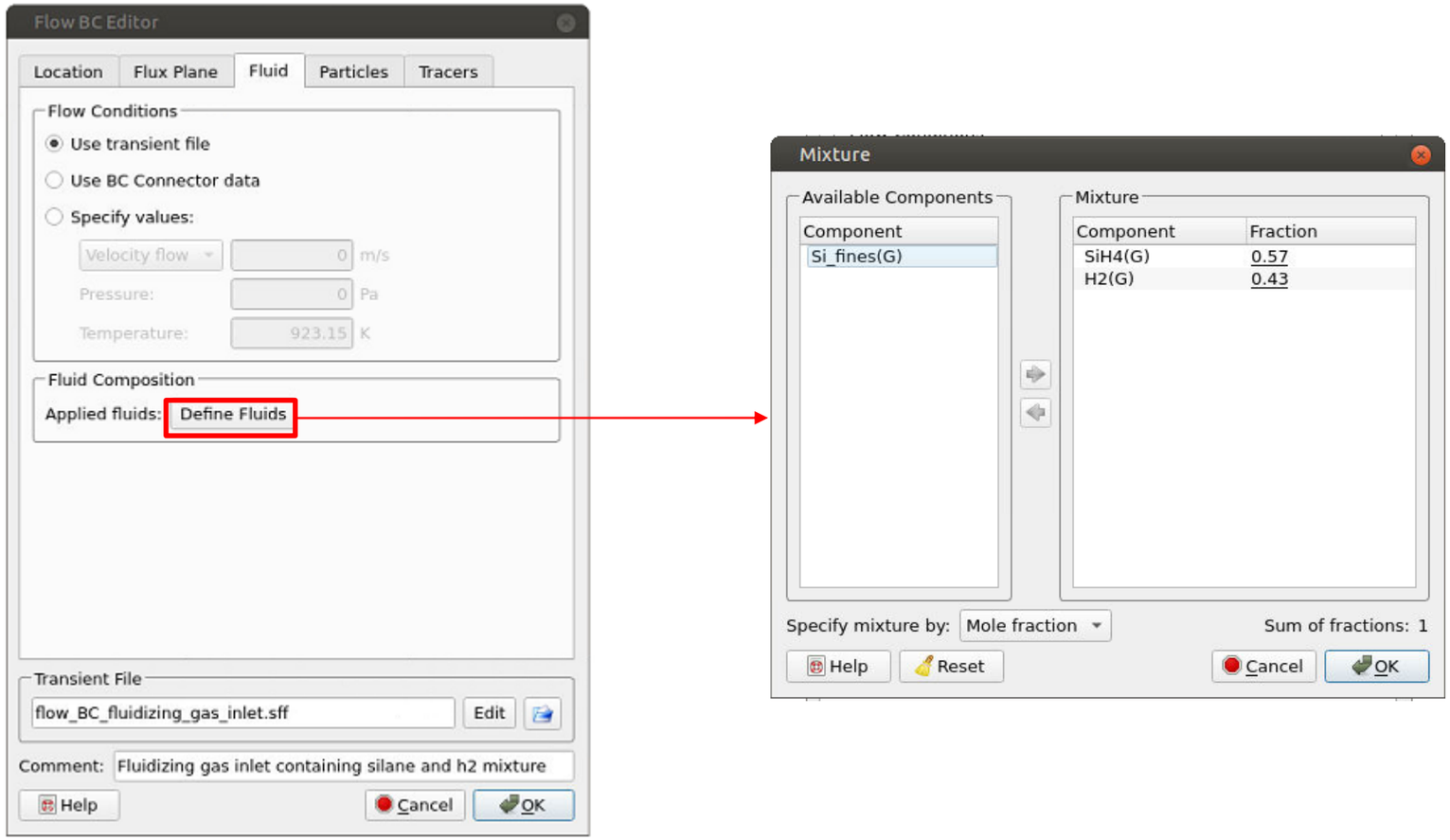
Flow BC will have a variable flow rate that is ramped up over 5 seconds

Enter a flow BC with the following conditions using a transient file



Flow BC

Use 0.57 mole fraction SiH4 and 0.43 mole fraction H2 under Defined Fluids.



Chemistry

The following reactions will be input into Barracuda. We will start by entering the appropriate reactions.

Reaction	Expression
Direct Deposition	$SiH_4 \rightarrow Si(s) + 2H_2$
Homogeneous Decomposition	$SiH_4 \rightarrow Si_{fines} + 2H_2$
Scavenging Reaction	$Si_{fines} \rightarrow Si(s)$

Kinetics

In the chemistry window under the Rate coefficients, we will enter the following rate coefficients:

Rate Coefficient	Rate Expression
k_{direct}	$2.793 * 10^{6}\ \theta_f^{-1}\ A_{Si}\ \exp\left(\frac{-19540}{T}\right)$
$k_{homogeneous}$	$2 * 10^{13} \exp\left(\frac{-26040}{T}\right)$
$k_{scavenging}$	$0.0071\ \theta_f^{-1} A_{Si}$

A_{Si}: refers to the surface area of Silicon particles divided by the cell volume ($\frac{m^2}{m^3}$).

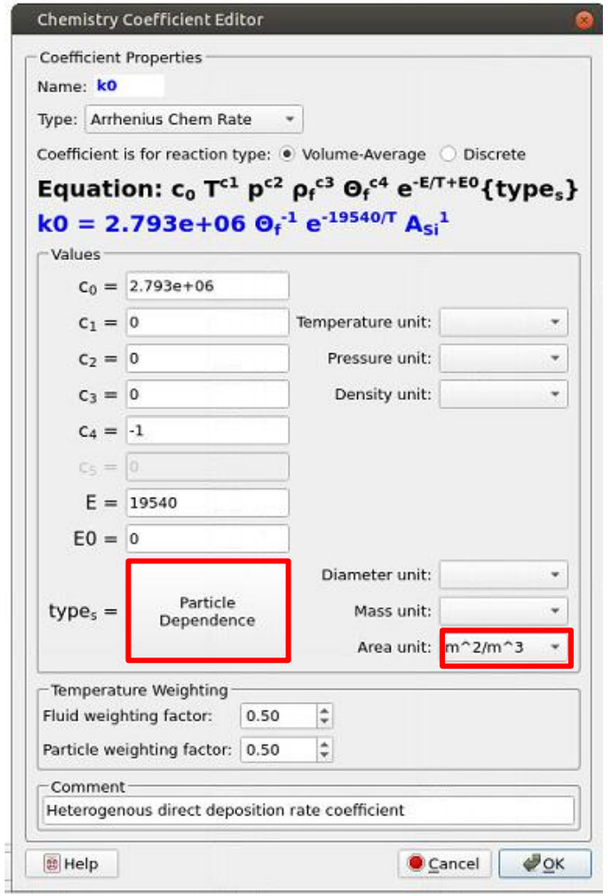
θ_f: fluid volume fraction

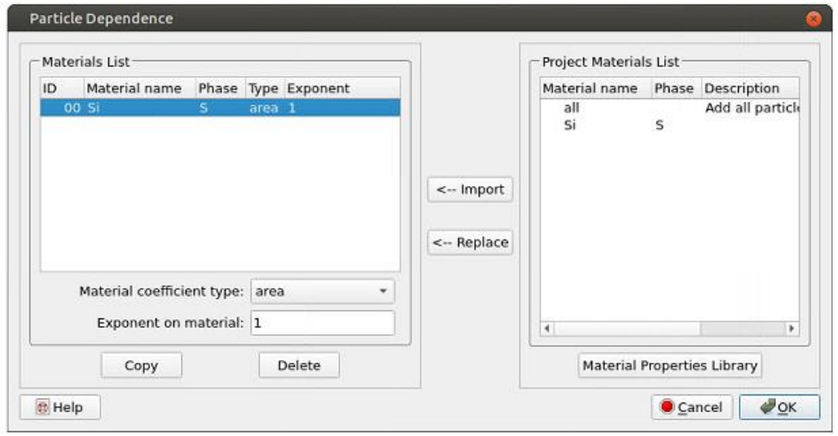
Kinetics

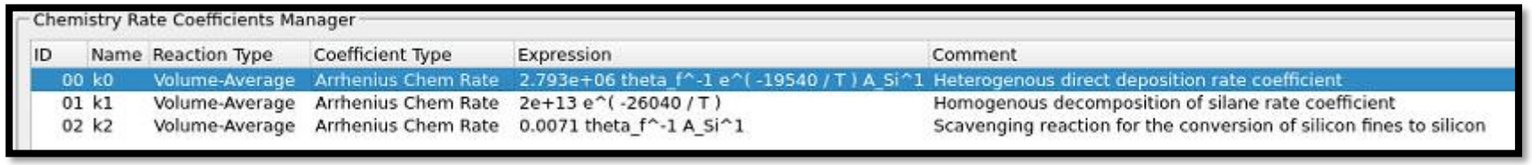
Define all rate coefficients:

Notes:

- For particle dependent properties (Silicon surface area), use the *Particle Dependence* button
- Create a new kinetic expression and select *Particle Dependence.*
- Import area with exponent defined as 1
- Define exponent c_4 as -1 for fluid volume fraction



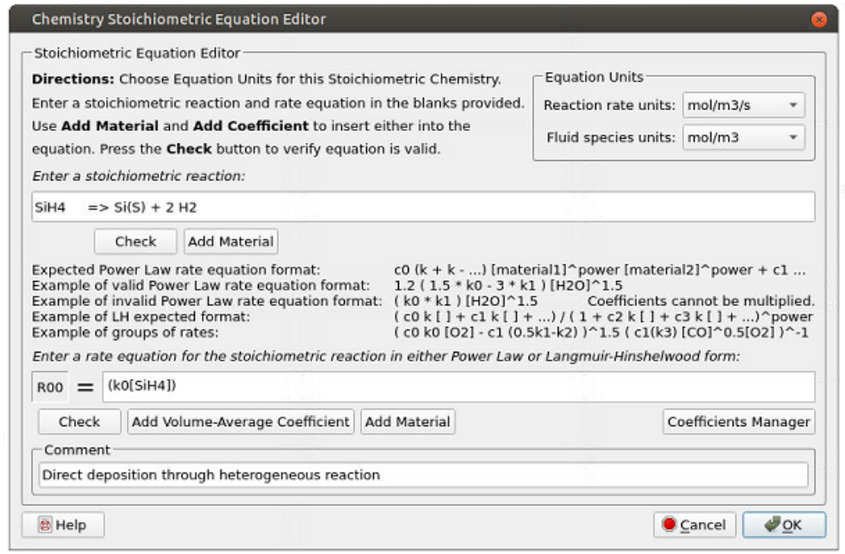


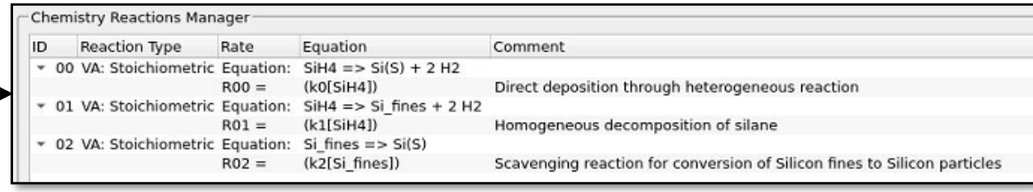


Chemistry

In the chemistry window under *Reactions*, select *Add* and enter the following Volume-averaged stoichiometric reactions.

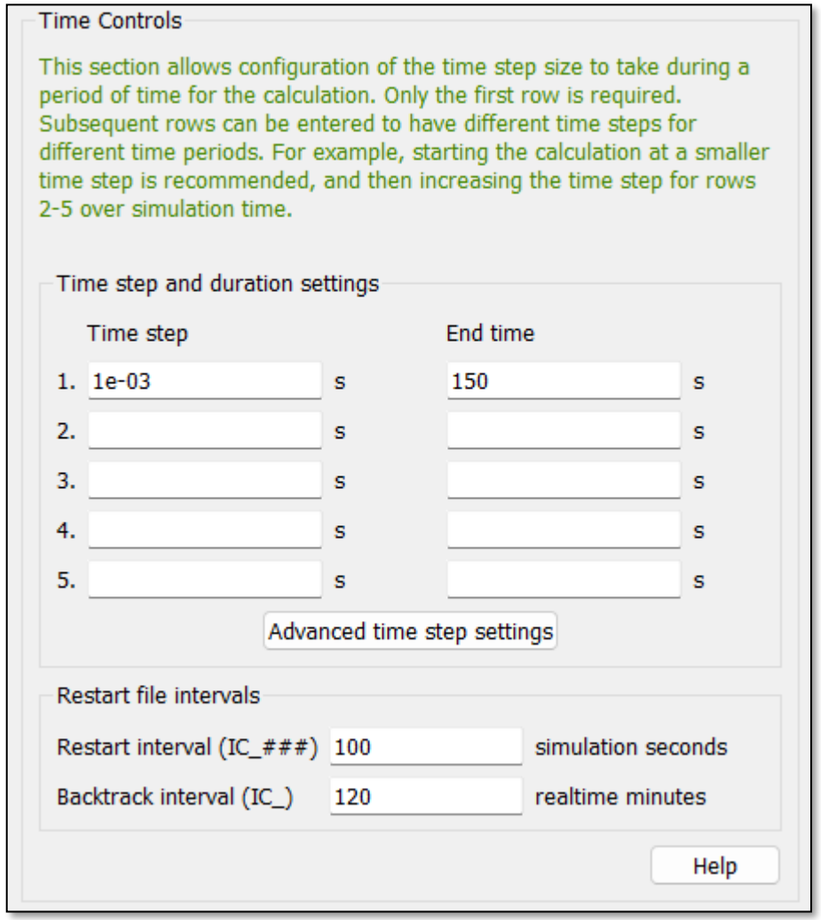
Reaction	Expression	Rate
Direct Deposition	$SiH_4 \rightarrow Si(s) + 2H_2$	$k_0[SiH_4]$
Homogeneous Decomposition	$SiH_4 \rightarrow Si_{fines} + 2H_2$	$k_1[SiH_4]$
Scavenging Reaction	$Si_{fines} \rightarrow Si(s)$	$k_2[Si\_fines]$





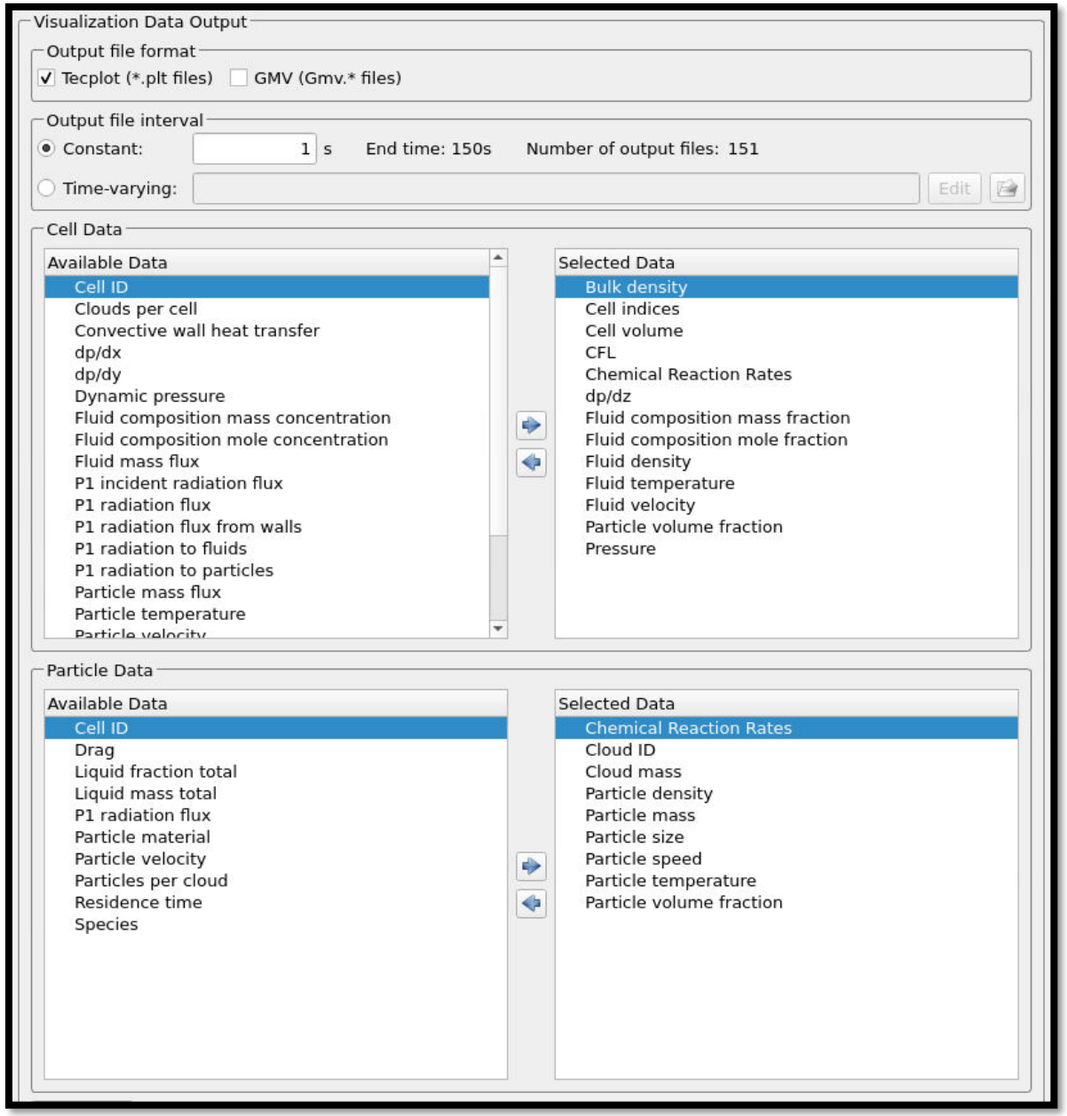
Time Controls

Set Time step and End time



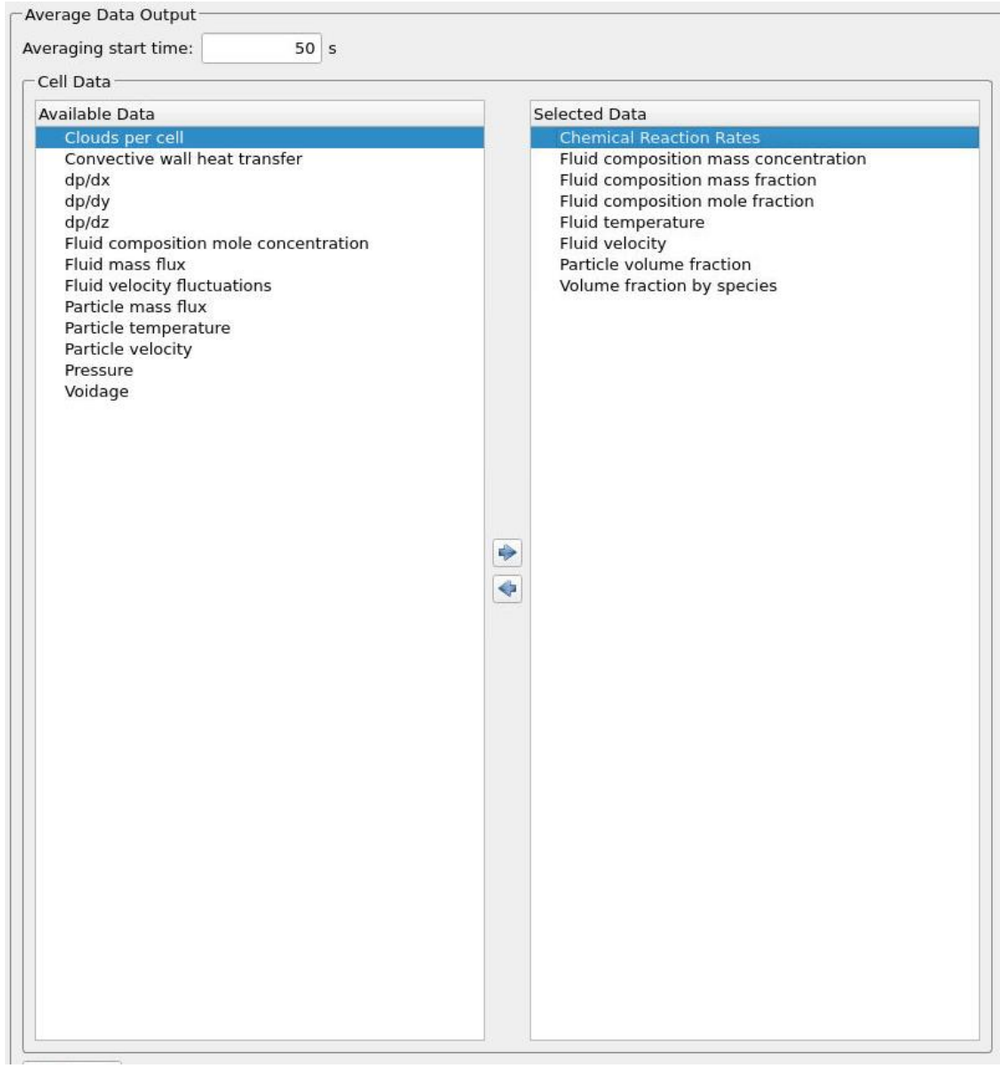
Visualization Data Output

Set Output file interval and select the options shown for Visualization Data Output.



Average Data Output

Select the following outputs under the Average Data window

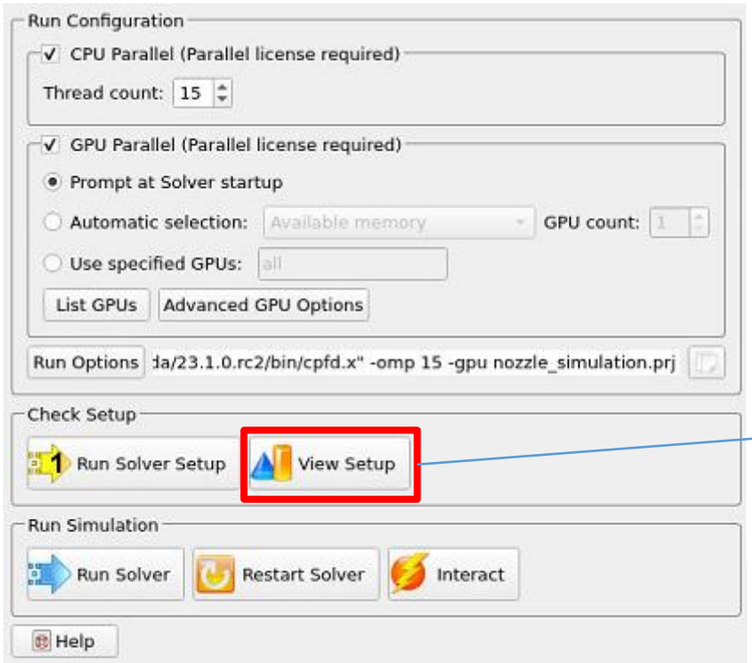


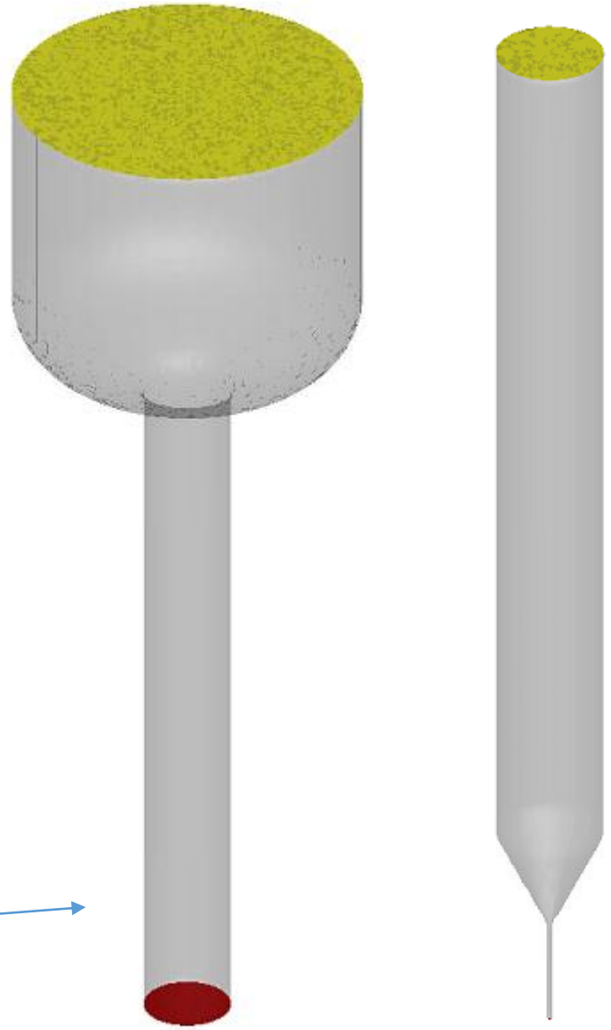
Run

If NVIDIA GPU card is available, select GPU Parallel

Run Solver Setup and View Setup

Once you have checked the setup, Run Solver to start the simulation



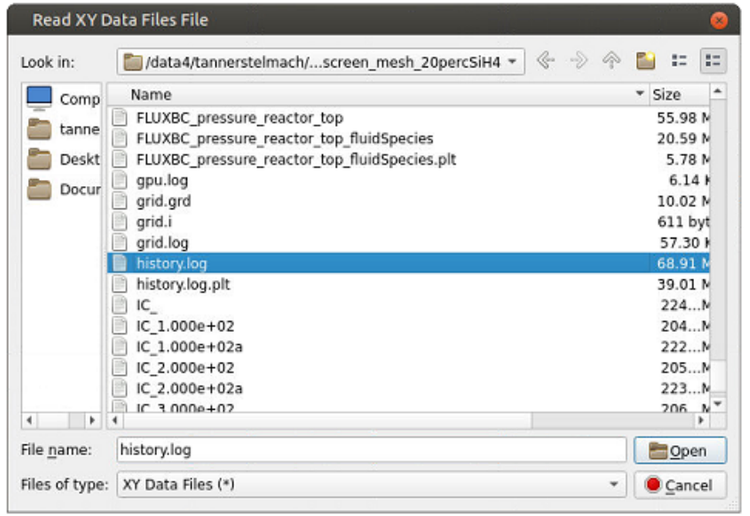


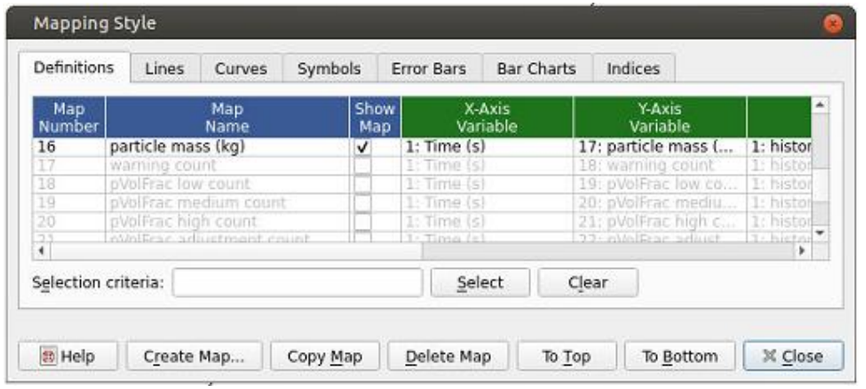
Post-Processing: Silicon Deposition Rate

To calculate the silicon deposition rate, we will use a linear fit to particle mass data. In the post-run window, select *Launch Tecplot:*

Select *File / Load Barracuda Data.* Select *Load Data File* and choose the *history.log* file.

Select *Mapping Style* and then change the output to output particle mass



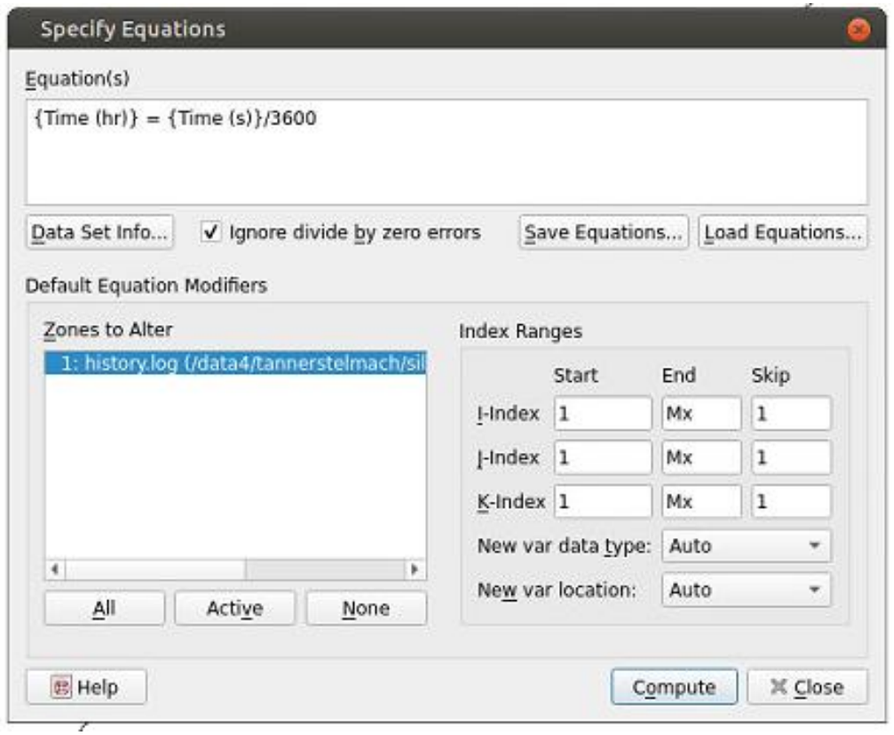


Post-Processing: Silicon Deposition Rate

The behavior of the plot is approximately linear. The deposition rate will be defined as the slope of this line

We need to plot particle mass (kg) with Time in *hours*, as our empirical data is reported in kg/hr.

Create a new *Time (hr)* variable using *Data / Alter / Specify Equations.* Enter the following expression. Select *Compute*



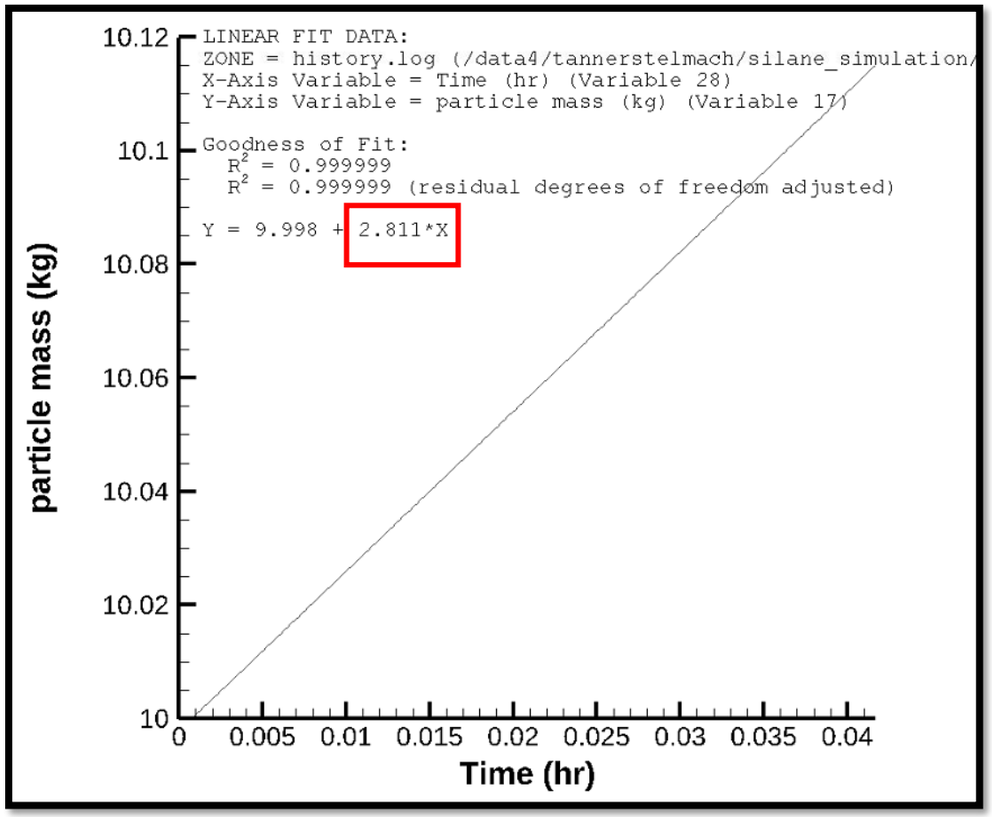
Post-Processing: Silicon Deposition Rate

Now, select *Mapping Style* and scroll to selected variable. Right click on the X-Axis Variable and change the variable to *Time (hr).*

Right click on the data line and select *Curve Type.* Choose *Linear Fit*

In the same window, select *Curve Details / Show on Plot.* The reported slope of the linear fit is the average deposition rate of silicon

This can optionally be repeated for all of the silicon fines results



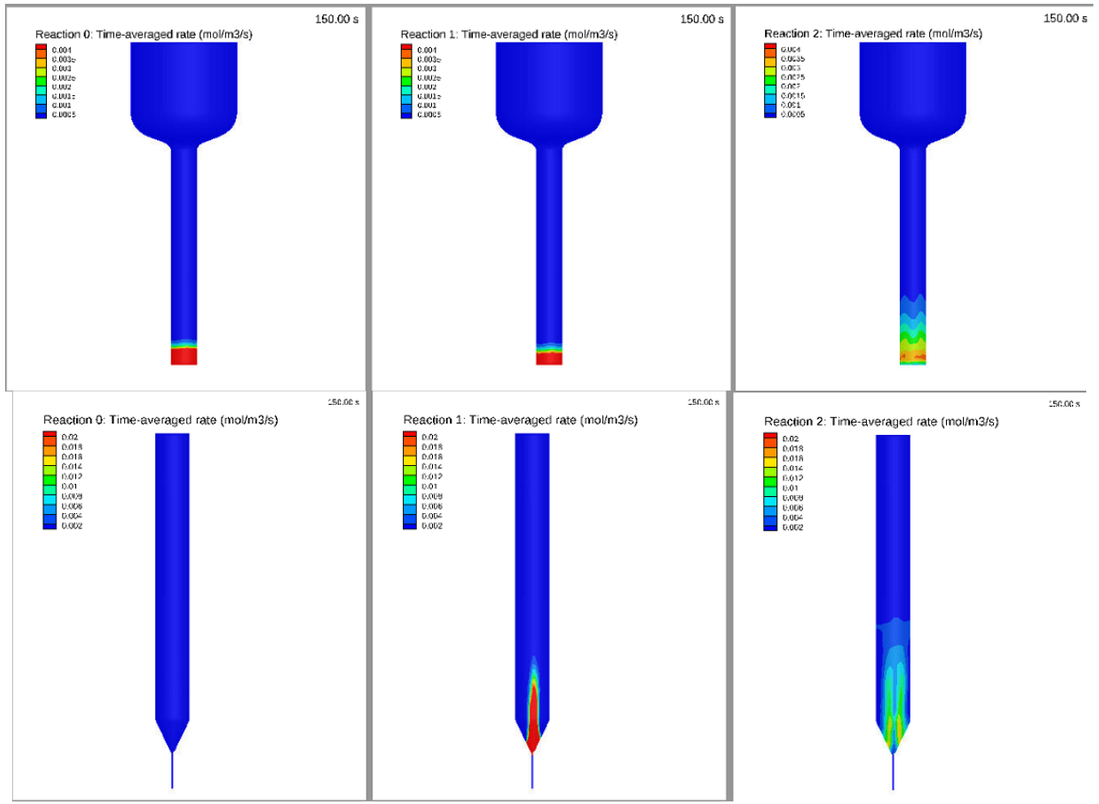
Post-Processing: Reaction Rate Output

Create a slice colored by Reaction rate

- Create a slice colored by time-averaged reaction rate to see the spatial variation in reaction rate for the system of interest

A video is included on how to make slices here:

https://cpfd-software.com/tecplot-for-barracuda-calculating-spatial-averages-on-slices/

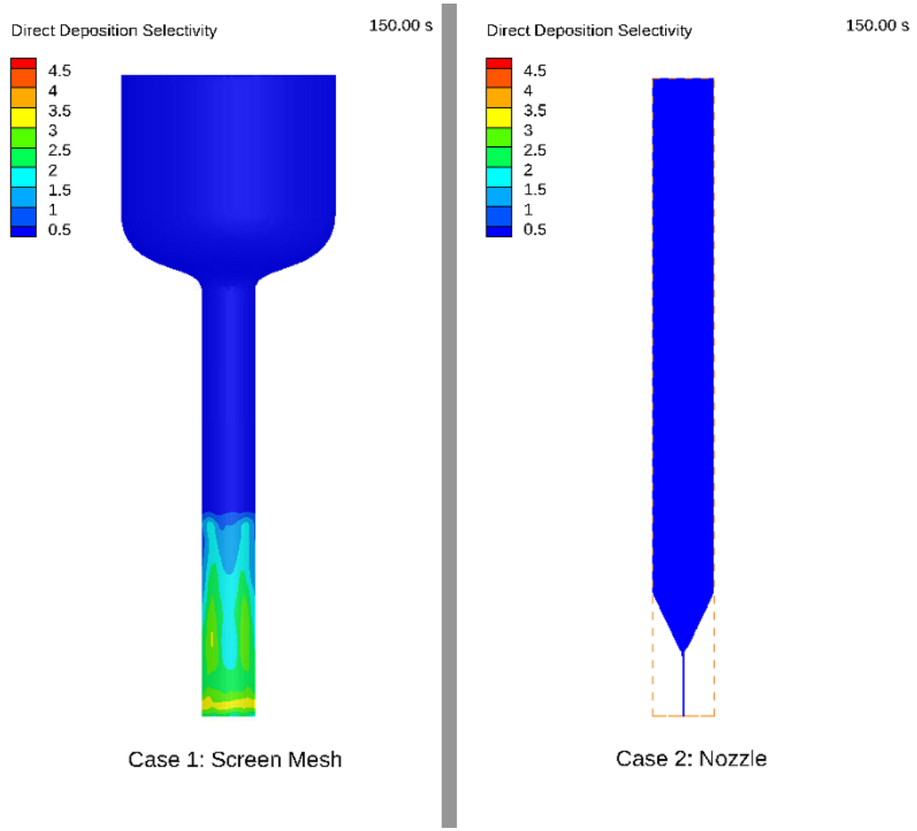


Post-Processing: Direct Deposition Reaction Selectivity

Reaction selectivity is a useful output to look at the favorability of certain reactions and is defined as the ratio of the rate of one reaction over another.

In this system, silicon fines are an undesired byproduct. We would like the direct deposition reaction to be favored over the production of silicon fines (an undesired byproduct).

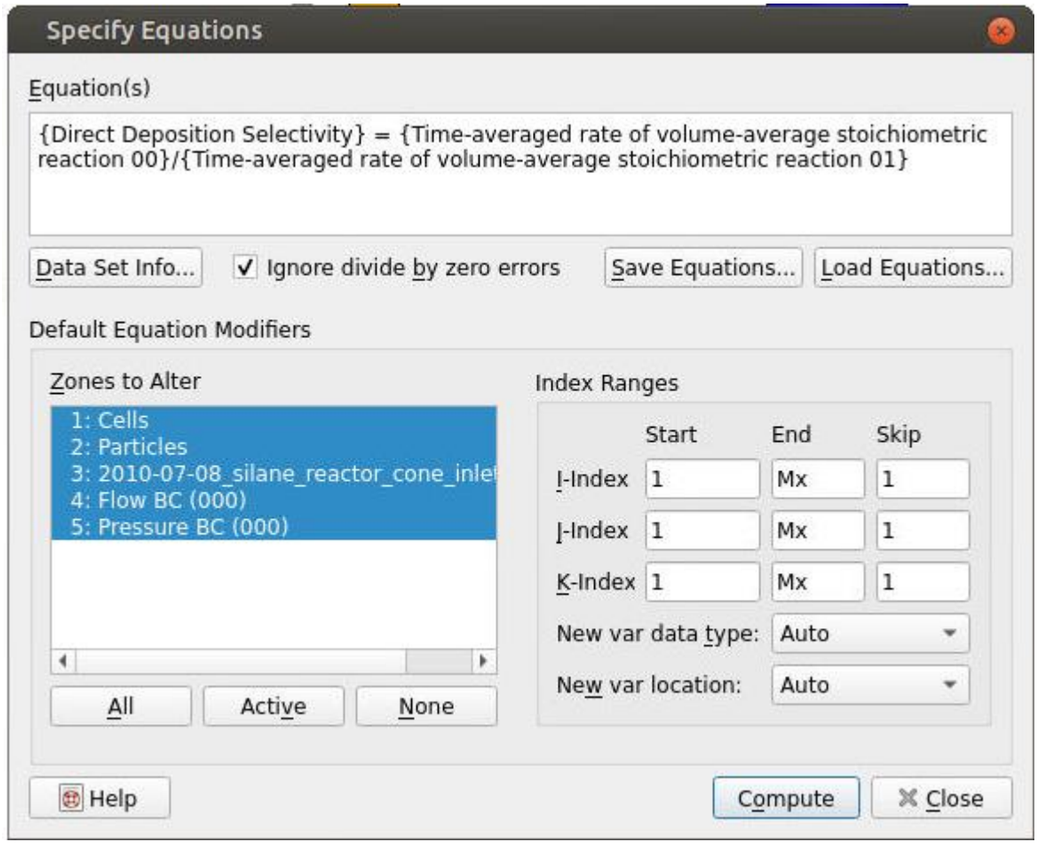
For our system, we would like the reaction selectivity of direct deposition to be high



Reaction selectivity output variable

The direct deposition reaction selectivity is defined as the ratio of the time-averaged rate of direct deposition and the time-averaged rate of the production of silicon fines. We will create a variable in Tecplot to visualize this

To do so, select *Data / Alter / Specify equation* and enter the following expression. Press *Compute*

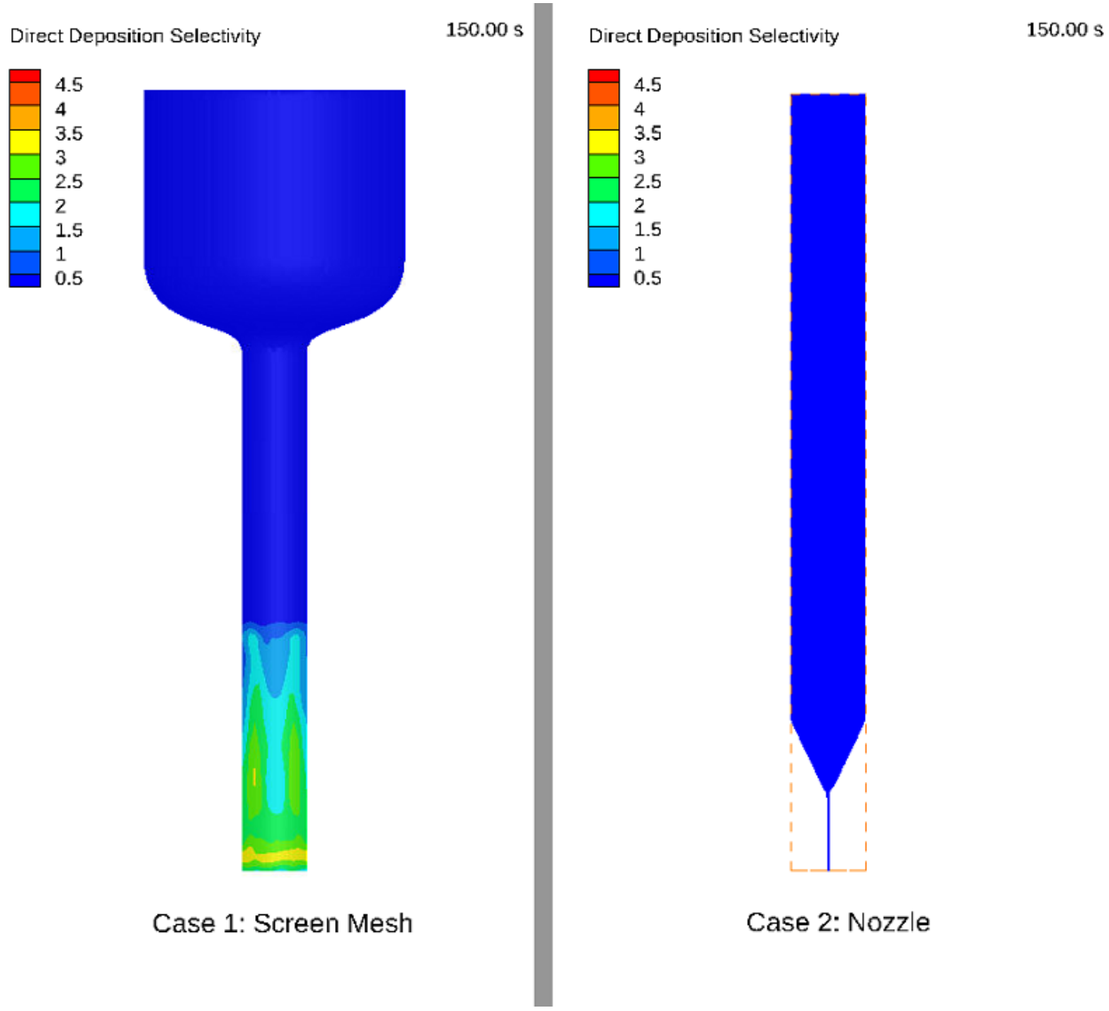


Create a slice and select the appropriate data

Double click the contour bar and select the drop-down menu. Select the variable that we just created (*Direct Deposition Selectivity).*

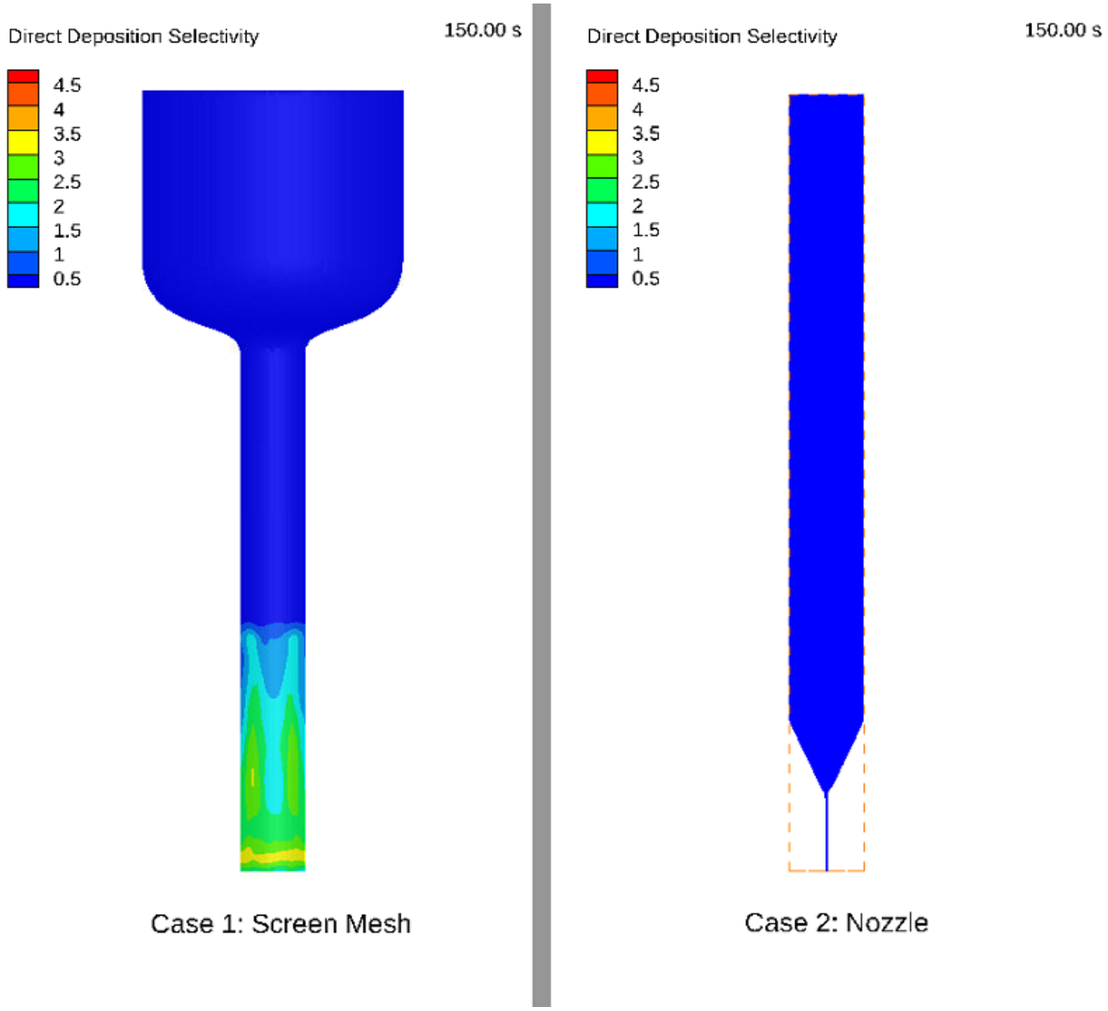
Adjust the color bar to the desired view. Here we use *Modified Rainbow (less green)*

Create a new frame, load Barracuda data from the nozzle simulation, and repeat the same steps to output reaction selectivity for the nozzle



Direct Deposition Rate Selectivity Conclusions

Results indicate that the screen mesh geometry has a higher average direct deposition reaction selectivity, which is preferred for silane deposition



Post-Processing: Silicon Fines Exit Mass Fraction

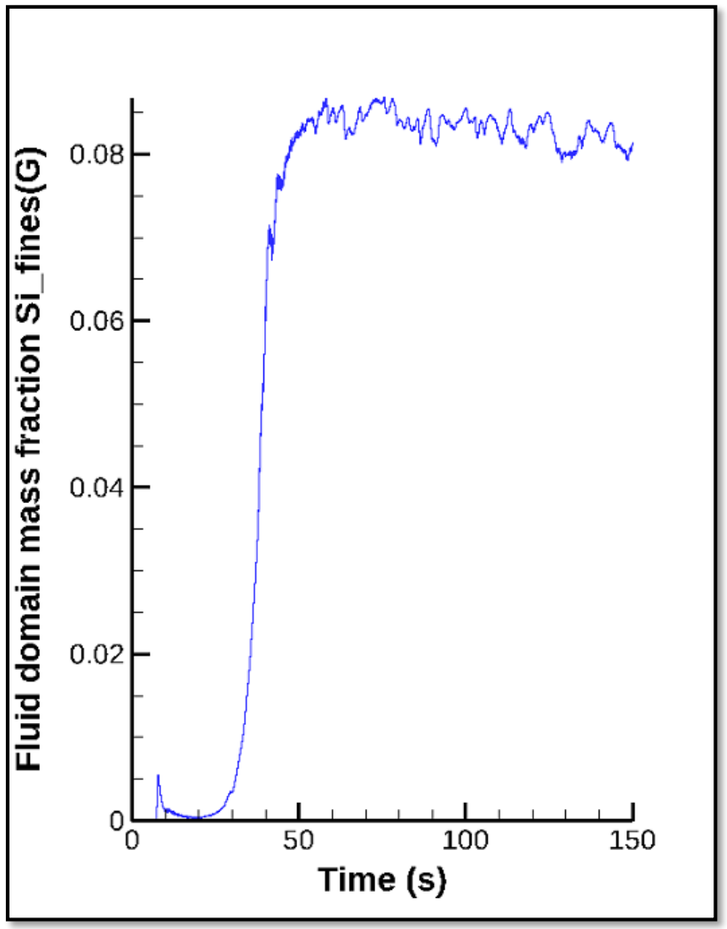
We would like to create a plot of the time-averaged mass fraction of silicon fines at the reactor exit.

First, select *Launch Tecplot,* then *File / Load Barracuda Data/ Load Data File/ FLUXBC_pressure_reactor_top_fluidSpecies.* This will open the Flux file at the reactor top

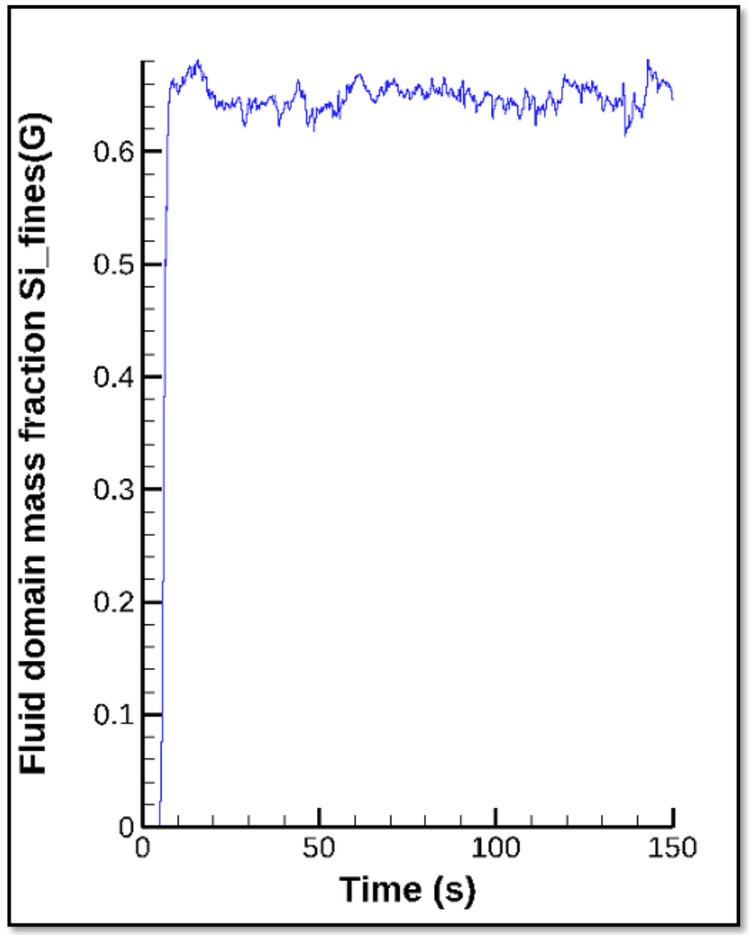
Post-Processing: Silicon Fines Exit Mass Fraction

Select mass fraction of Silicon Fines from the variable selection menu to generate the following plot for the nozzle and screen mesh geometry

Screen Mesh



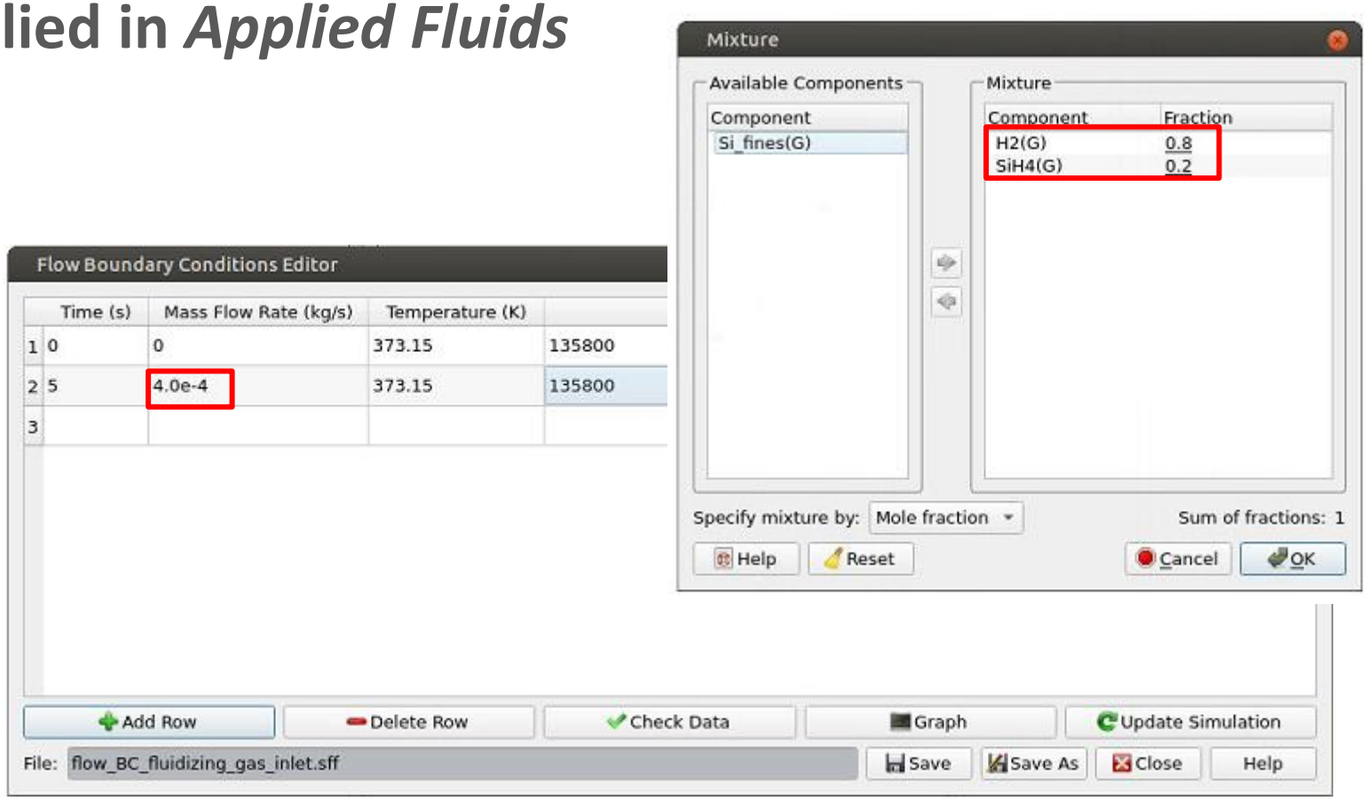
Nozzle



Other cases (optional)

Experimental results are available at different silane feed fractions (20%, 50%, and 80% mole fraction SiH_4). These can be explored by modifying the Flow BC sff file to account for the correct flowrate. These are listed here. Ensure that the appropriate mole fraction is applied in *Applied Fluids*

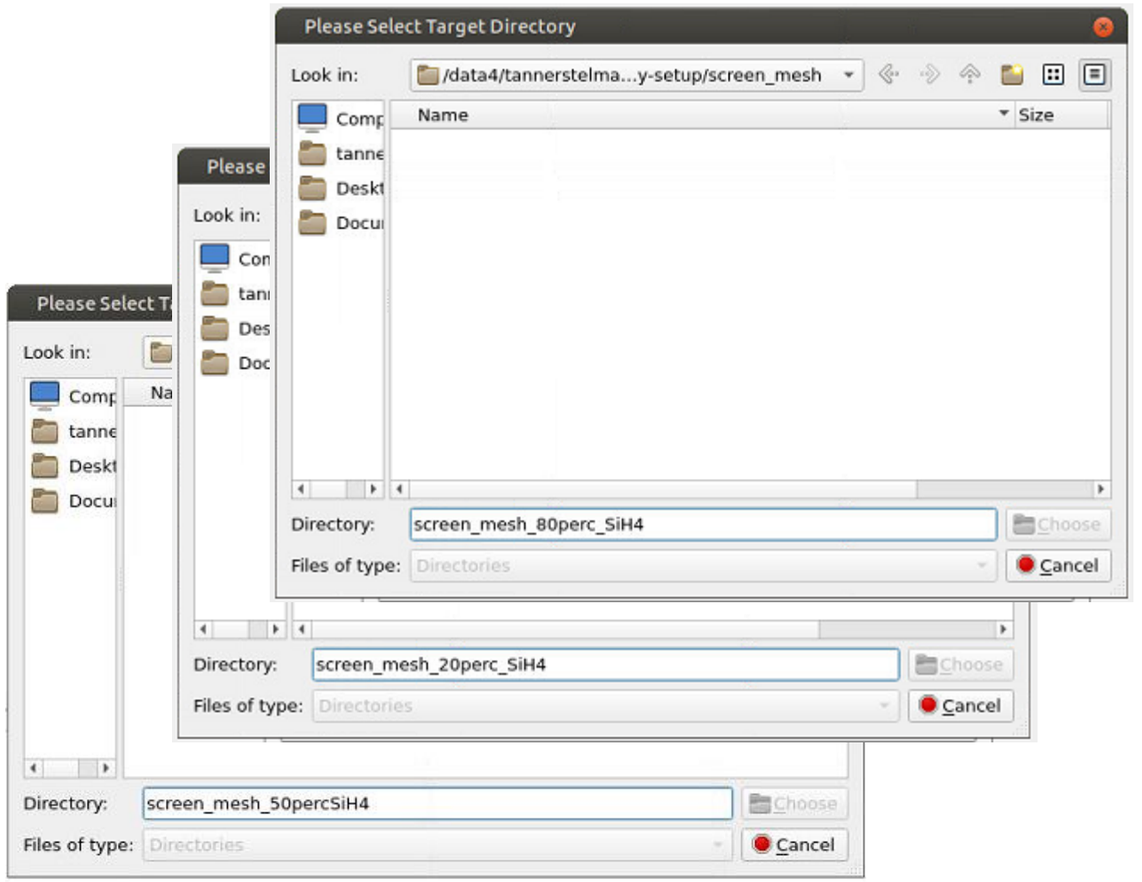
Mole Fraction SiH4 (mol%)	Flowrate (kg/s)
20%	4.0e-04
50%	8.5e-04
80%	1.3e-03



Test other feed fractions of SiH4 using Save Case As

From the original project files, select *File / Save Case As* and select appropriate directory (screen_mesh or nozzle)

Save file names with the mole fraction included in the file name. Do this for a mole fraction of **20, 50, and 80% SiH4**



Post-Processing: Silicon Deposition Rate (optional)

Follow steps for all four cases with analysis of the silicon deposition rate, and silicon fines production. Simulation results can be compared with the empirical data from James Parker 2011 shown here:

Experimental Results (Parker 2011)		
Silane Feed Mole Fraction	Deposition Rate (kg/hr)	Si_fines Mass Fraction at Reactor Exit
20%	1	3.9
50%	2.4	--
57%	3	9.4
80%	3.5	11.4

Summary

This model showed an example of a CFD simulation based on a real industrial application.

Post-processing was done to compare the rate of direct deposition and silicon fines production

Comparison of deposition rate, silicon fines production, and reaction selectivity of direct deposition showed advantage of screen mesh configuration

System Pressure: 1.358 bar