

Silane Deposition: Setup and Analysis

CPFD Software

www.cpfd-software.com

Silane Deposition

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

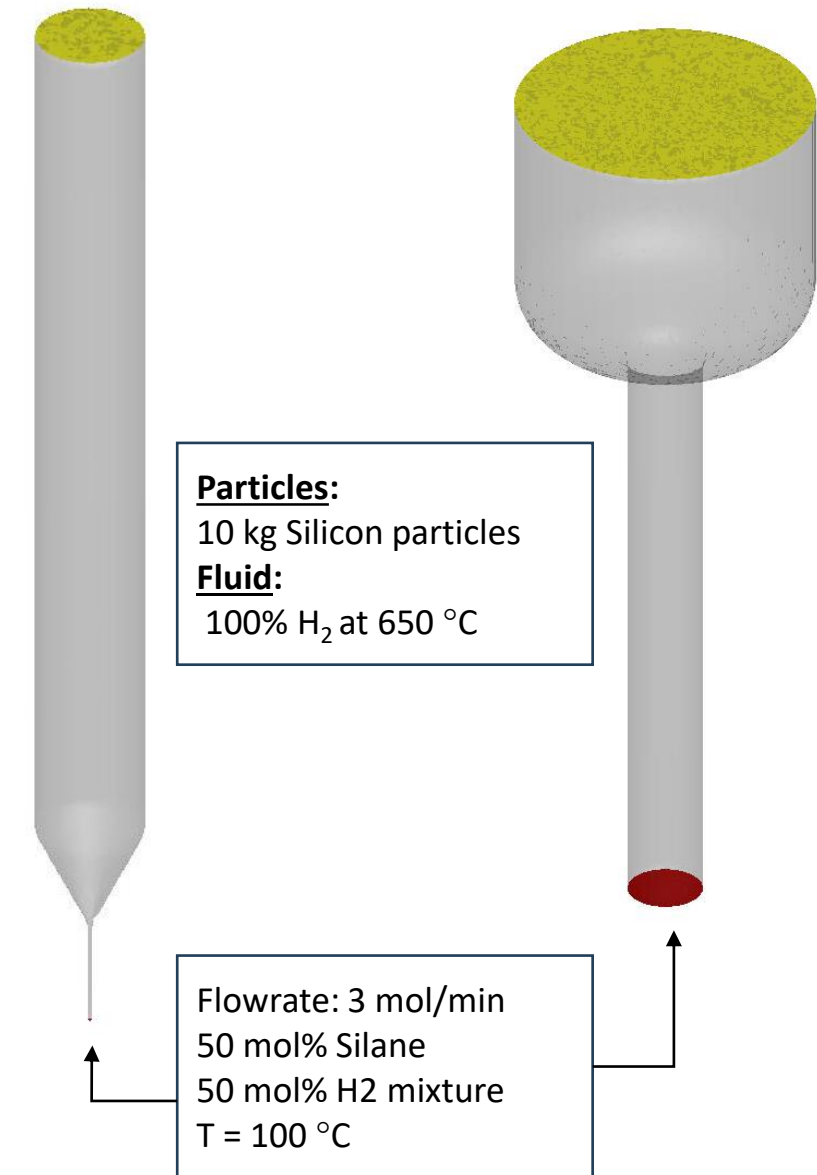
Case 1: Screen Mesh

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

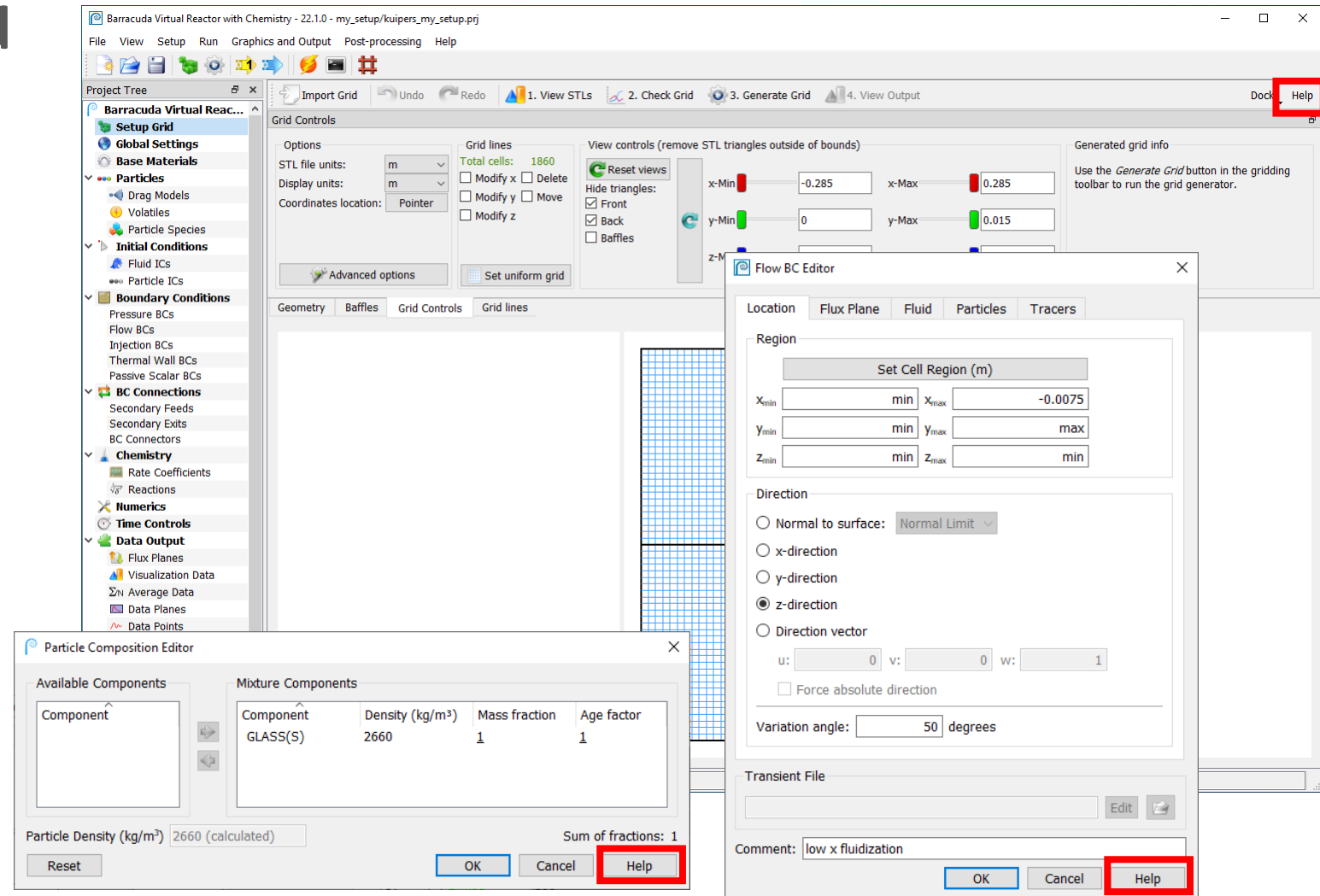
System Pressure: 1.358 bar



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

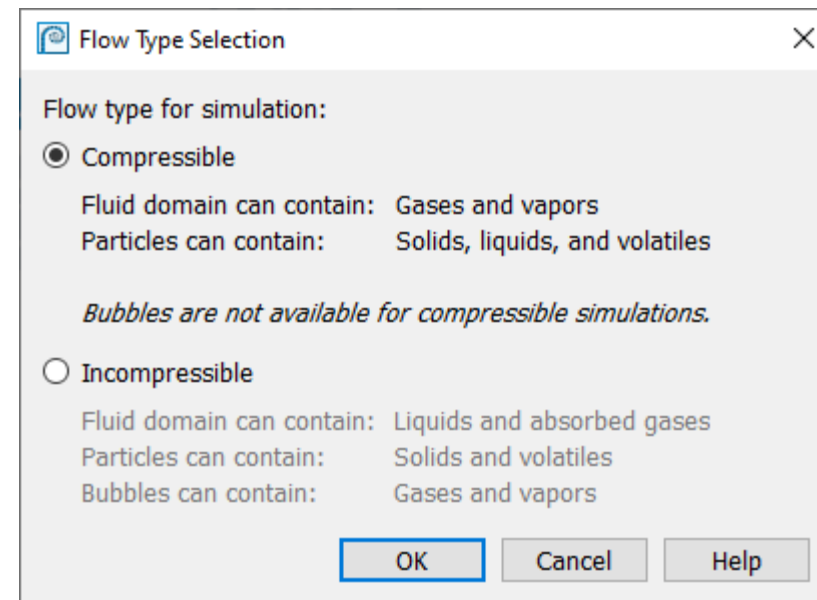
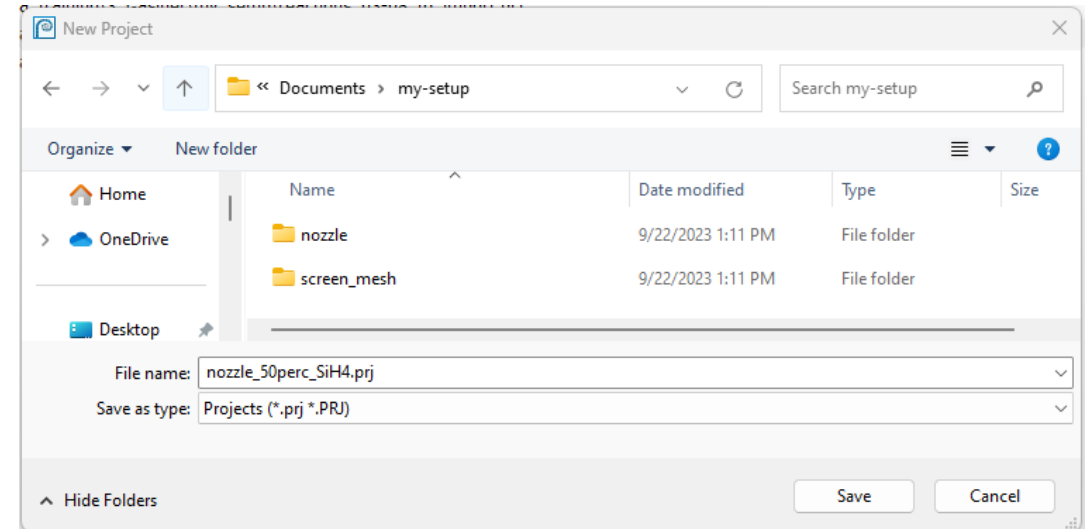
my-setup\nozzle\57perc_SiH₄

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

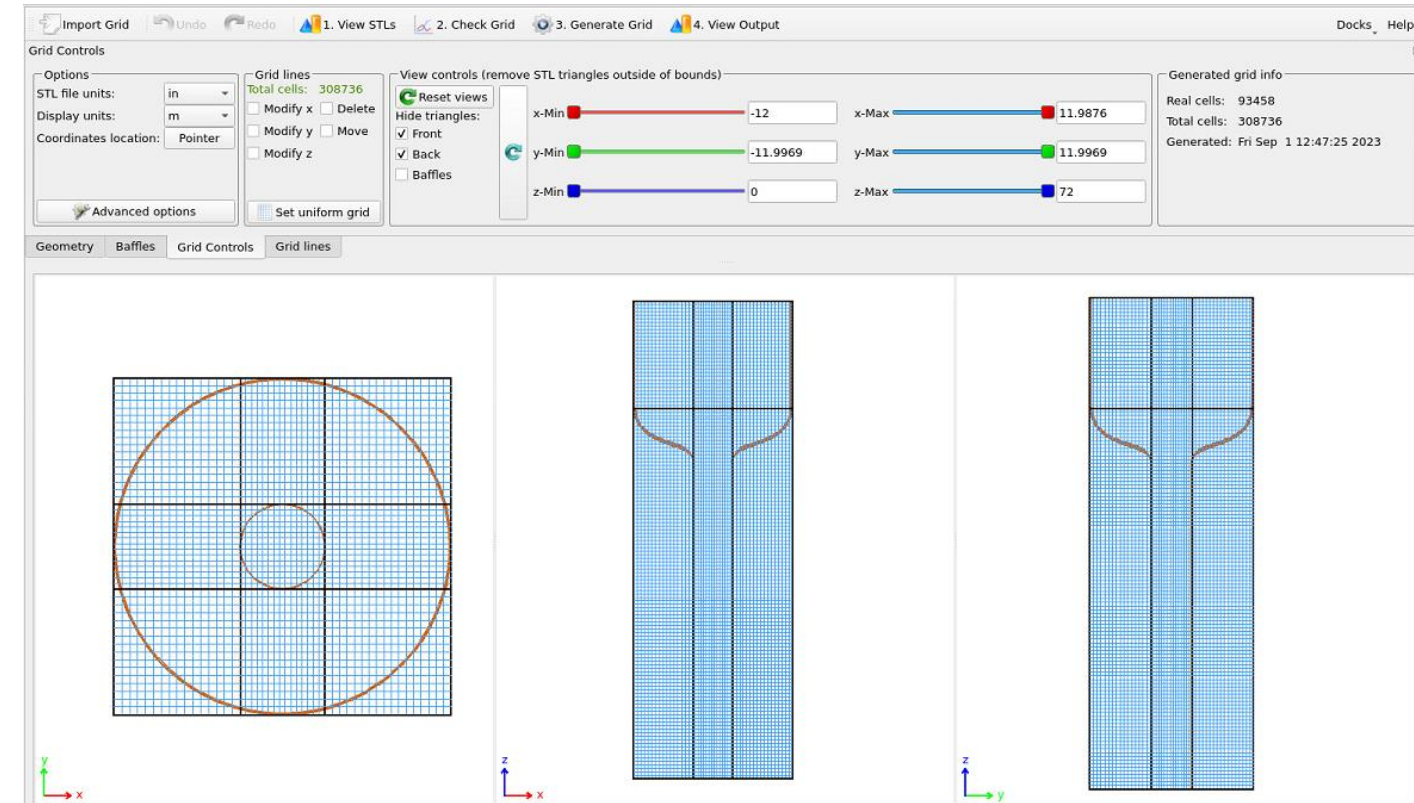
In the
`screen_mesh/screen_mesh_57perc_SiH4.prj` file

Geometry tab:

- Add 2010-07-02_silane_reactor_flat_inlet.stl

Controls tab:

- Set STL file units to inches



Nozzle: Setup Grid

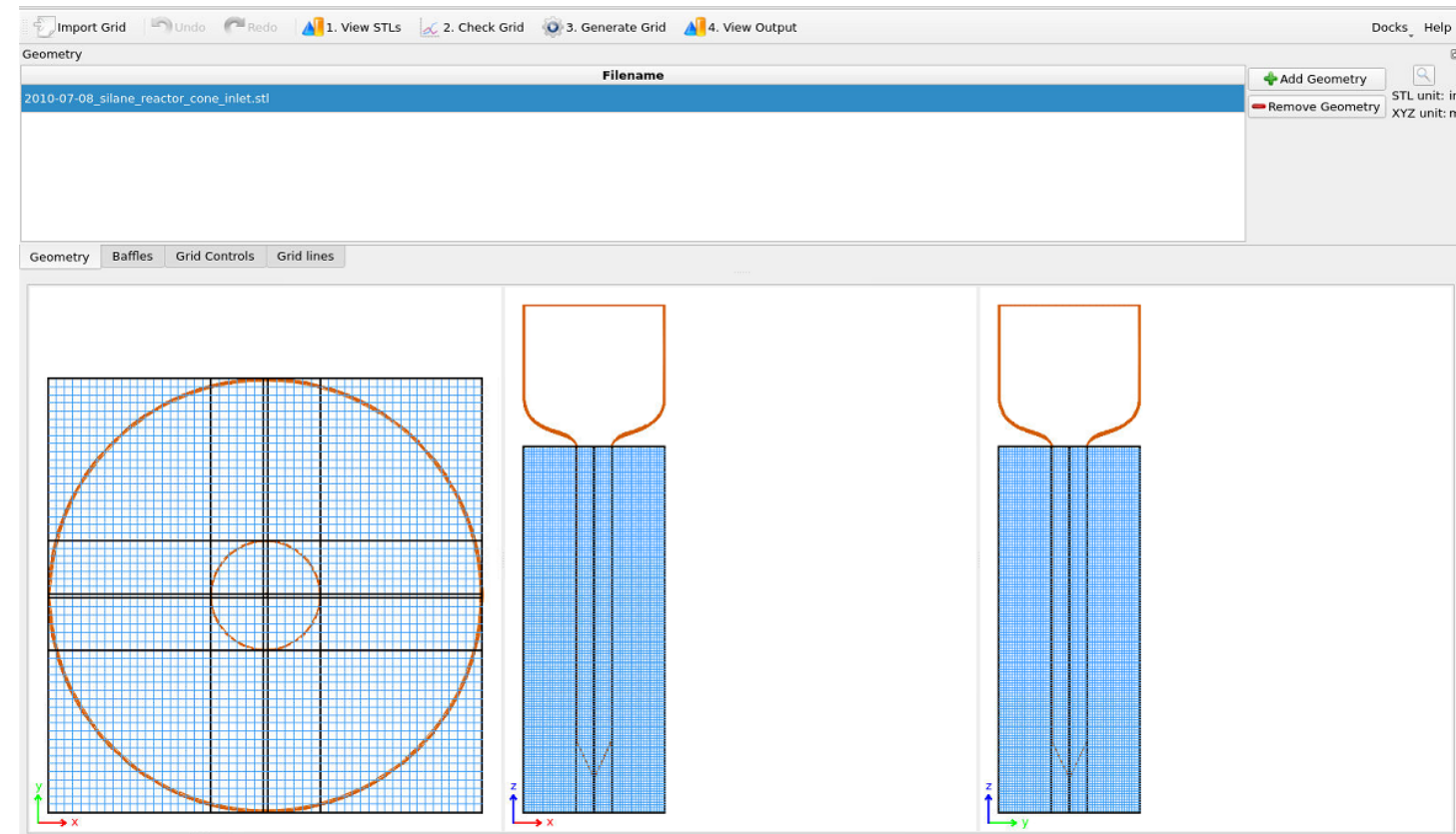
In the **nozzle/nozzle_57perc_SiH4.prj** file

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

Global Settings

Flow Type: Compressible

Fluid domain can contain: Gases and vapors

Particles can contain: Solids, liquids, and volatiles

Bubbles are not available for compressible simulations.

Gravity Settings

x-direction: m/s² y-direction: m/s² z-direction: m/s²

Thermal Settings

☐ Isothermal

Temperature: K

☒ Thermal

Heat Transfer Coefficients

Radiation Model


☒ None ☐ Near wall ☐ P-1 ☒ Cap exposed particle area

Temperature Warning Limits

Minimum: K Maximum: K

☐ Record minimum and maximum temperatures in MinMaxTemp.data log file

Simulation Start Options

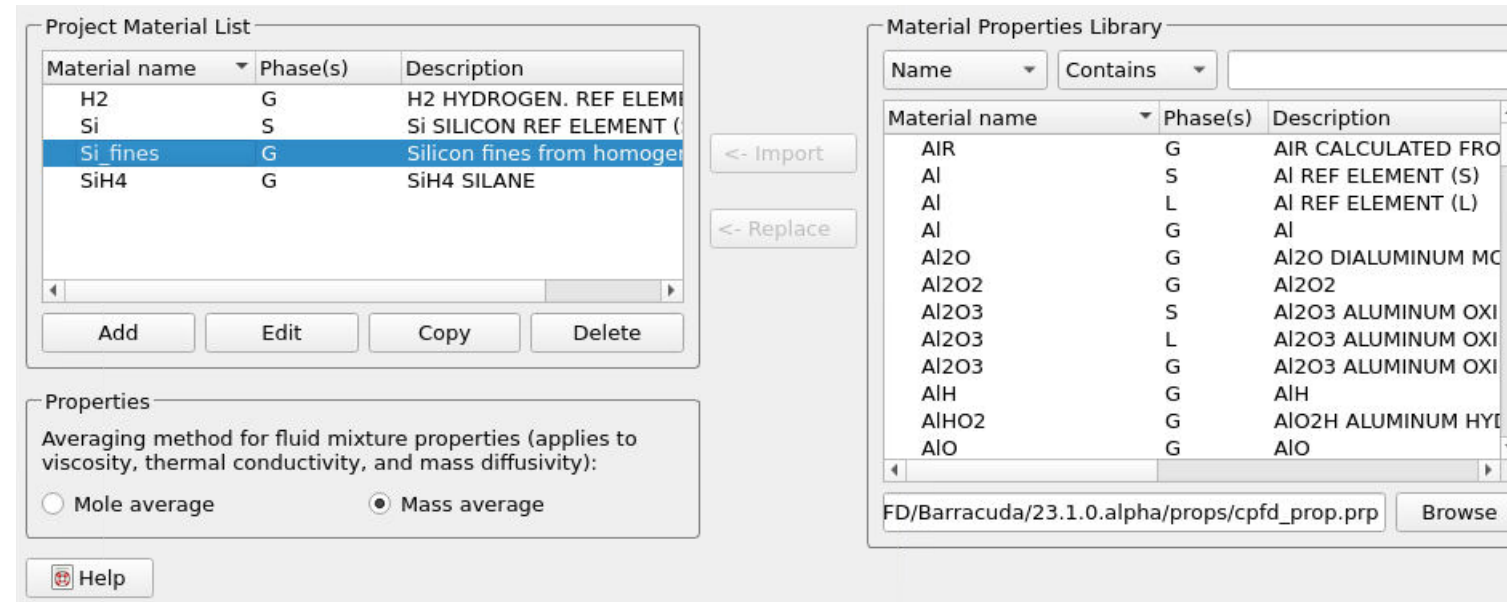
 Help

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 = $3\text{e-}5 \text{ Pa}\cdot\text{s}$

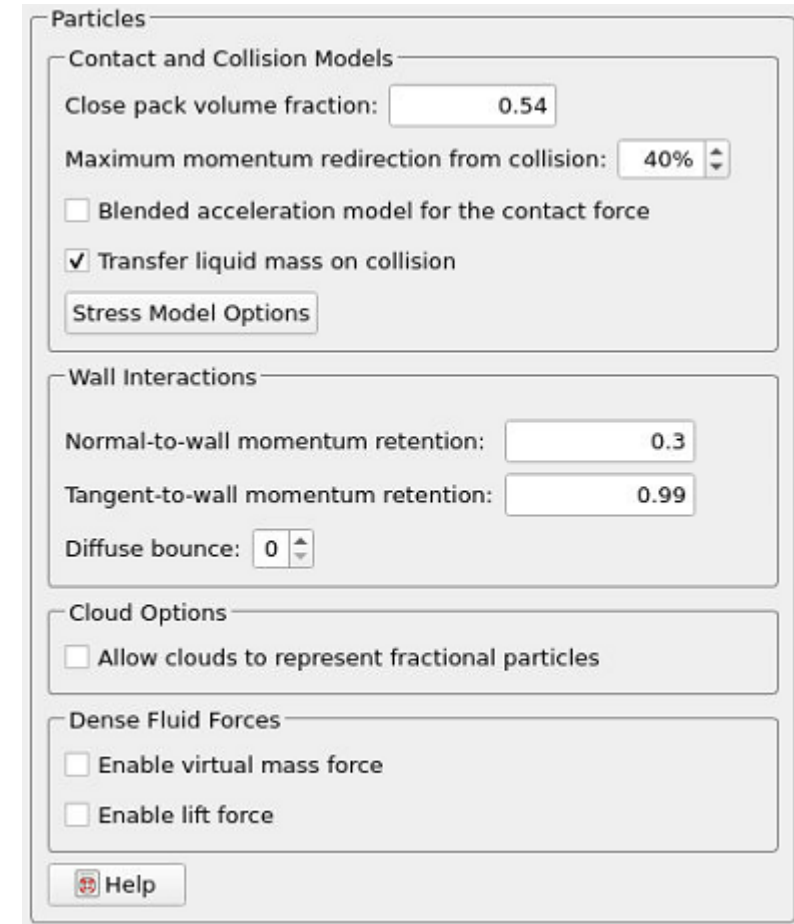


Particles

Set Close pack volume fraction: 0.54

Normal-to-wall momentum retention: 0.3

Tangent-to-wall momentum retention: 0.99



The screenshot shows the 'Particles' settings panel with the following configuration:

- Contact and Collision Models**
 - Close pack volume fraction: 0.54
 - Maximum momentum redirection from collision: 40%
 - ☐ Blended acceleration model for the contact force
 - ☒ Transfer liquid mass on collision
 - Stress Model Options
- Wall Interactions**
 - Normal-to-wall momentum retention: 0.3
 - Tangent-to-wall momentum retention: 0.99
 - Diffuse bounce: 0
- Cloud Options**
 - ☐ Allow clouds to represent fractional particles
- Dense Fluid Forces**
 - ☐ Enable virtual mass force
 - ☐ Enable lift force
- Help

Particles Species

Create a Silicon particle species with the following properties:

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

Particle Species Manager							
Species-ID	Comment	Materials	Size	Sphericity	Emissivity	Drag model	Agglomeration
001	Silicon p...	Si	7...	1	1	WenYu-Erg...	Off

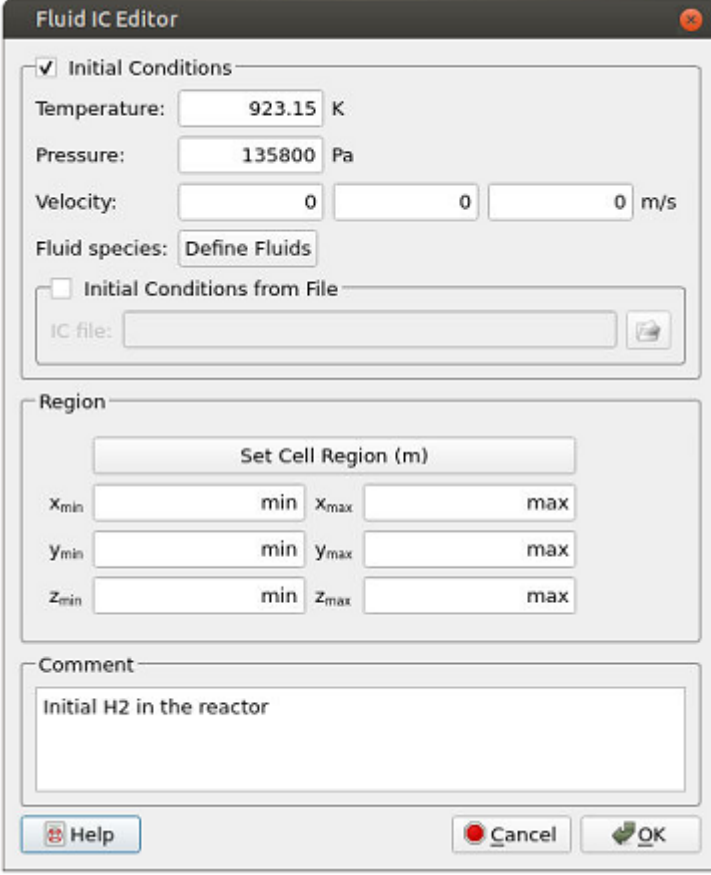
Screen Mesh: Fluid and Particle ICs

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



Fluid IC Editor

☒ Initial Conditions

Temperature: 923.15 K

Pressure: 135800 Pa

Velocity: 0 0 0 m/s

Fluid species: Define Fluids

☐ Initial Conditions from File

IC file:

Region

Set Cell Region (m)

X_{min} min X_{max} max

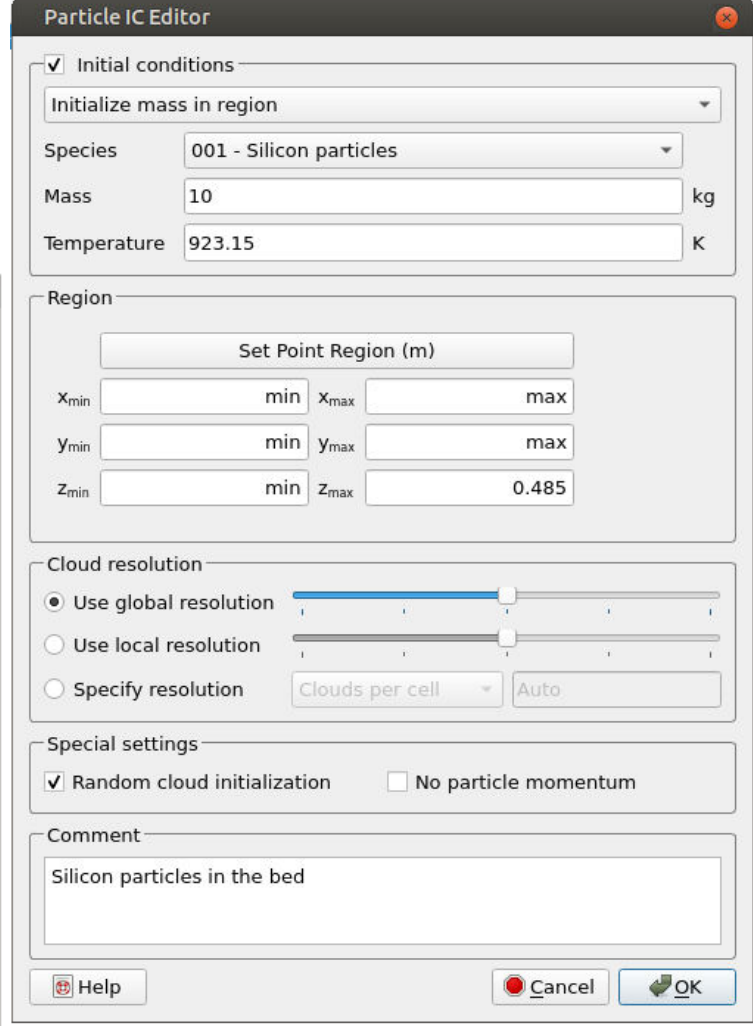
Y_{min} min Y_{max} max

Z_{min} min Z_{max} max

Comment

Initial H2 in the reactor

Help Cancel OK



Particle IC Editor

☒ Initial conditions

Initialize mass in region

Species: 001 - Silicon particles

Mass: 10 kg

Temperature: 923.15 K

Region

Set Point Region (m)

X_{min} min X_{max} max

Y_{min} min Y_{max} max

Z_{min} min Z_{max} 0.485

Cloud resolution

☒ Use global resolution

☐ Use local resolution

☐ Specify resolution Clouds per cell Auto

Special settings

☒ Random cloud initialization ☐ No particle momentum

Comment

Silicon particles in the bed

Help Cancel OK

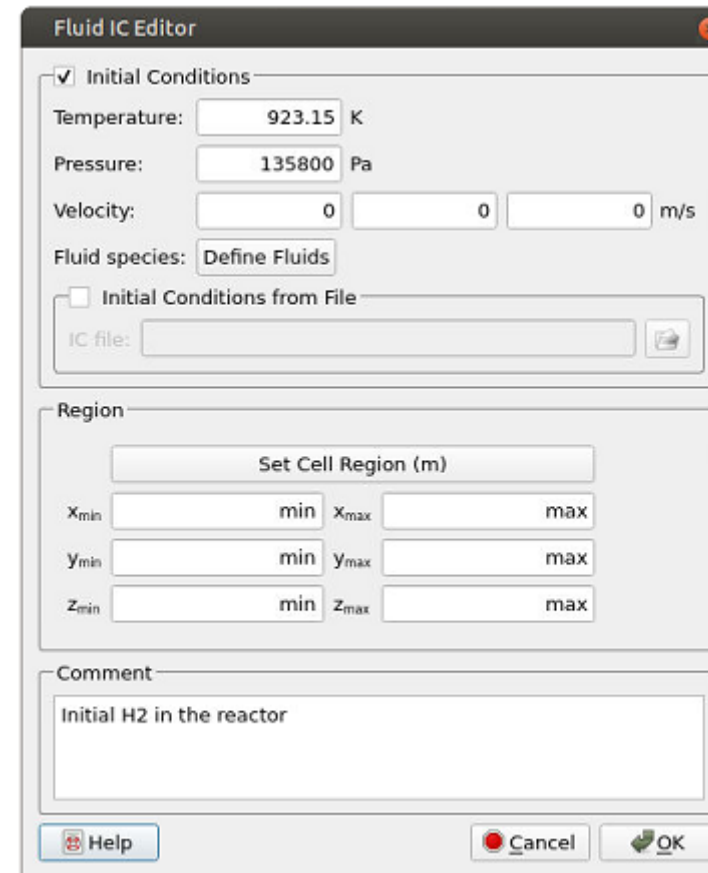
Nozzle: Fluid and Particle ICs

Fluid IC

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

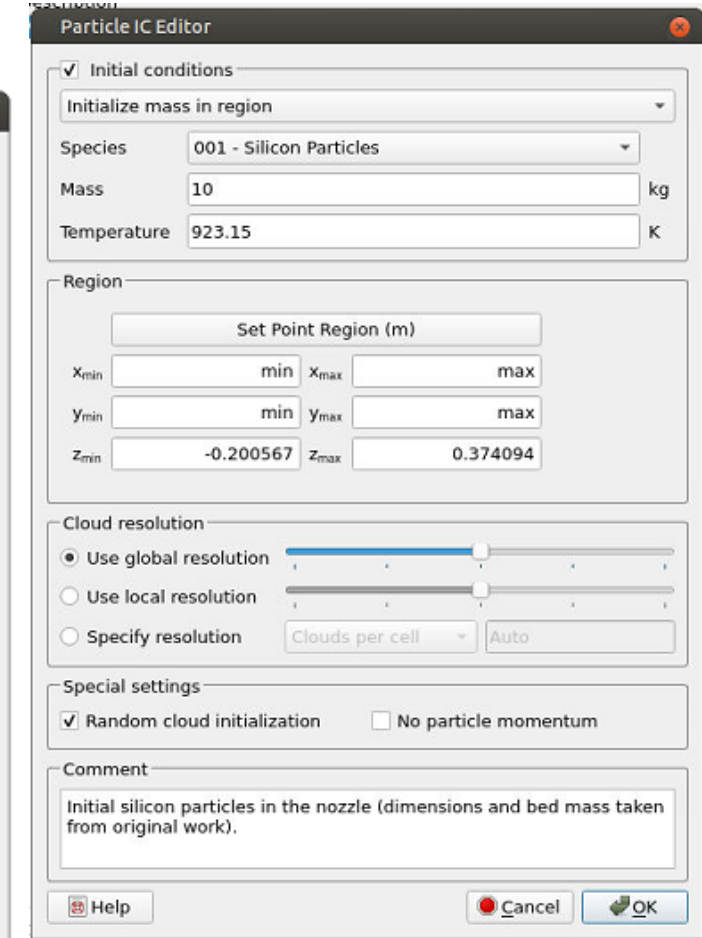
Particle IC

- 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



The Fluid IC Editor dialog box is shown with the following settings:

- ☒ Initial Conditions
- Temperature: 923.15 K
- Pressure: 135800 Pa
- Velocity: 0 0 0 m/s
- Fluid species: Define Fluids
- ☐ Initial Conditions from File
- IC file: (empty)
- Region: Set Cell Region (m)
 - Xmin: min Xmax: max
 - Ymin: min Ymax: max
 - Zmin: min Zmax: max
- Comment: Initial H2 in the reactor
- Buttons: Help, Cancel, OK



The Particle IC Editor dialog box is shown with the following settings:

- ☒ Initial conditions
- Initialize mass in region (dropdown)
- Species: 001 - Silicon Particles
- Mass: 10 kg
- Temperature: 923.15 K
- Region: Set Point Region (m)
 - Xmin: min Xmax: max
 - Ymin: min Ymax: max
 - Zmin: -0.200567 Zmax: 0.374094
- Cloud resolution:
 - ☒ Use global resolution
 - ☐ Use local resolution
 - ☐ Specify resolution: Clouds per cell (dropdown), Auto (button)
- Special settings:
 - ☒ Random cloud initialization
 - ☐ No particle momentum
- Comment: Initial silicon particles in the nozzle (dimensions and bed mass taken from original work).
- Buttons: Help, Cancel, OK

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:

Pressure Boundary Conditions Editor

	Time (s)	Pressure (Pa)	Temperature (K)	Area Fraction	Particle Feed	K-Factor
1	0	135000	923.15	1	<input type="radio"/> Off	0
2					<input checked="" type="radio"/> On	

File: pressure_BC_5psig.sff

Buttons: Add Row, Delete Row, Check Data, Graph, Update Simulation, Save, Save As, Close, Help

Pressure BC Editor

Location Flux Plane Fluid Particles Tracers

Region

Set Cell Region (m)

X_{min} min X_{max} max

Y_{min} min Y_{max} max

Z_{min} max Z_{max} max

Direction

☐ x-direction

☐ y-direction

☒ z-direction

Comment: Top of reactor boundary condition

Buttons: Help, Cancel, OK

Pressure BC Editor

Location Flux Plane Fluid Particles Tracers

Name: FLUXBC_pressure_reactor_top

Fluid species behavior:

Mass time cumulative

☐ Bin by particle size 100 bins

☐ Output raw particle data

☐ Output tracer data

Comment: Top of reactor boundary condition

Buttons: Help, Cancel, OK

Pressure BC Editor

Location Flux Plane Fluid Particles Tracers

Flow Conditions

☒ Transient file:

pressure_BC_5psig.sff Edit

☐ Specify values:

Area fraction: 1

Pressure: 0 Pa

Temperature: 923.15 K

K-factor: 0

Fluid Composition

Fluid inflow properties: Interior cell values

Applied fluids: Define Fluids

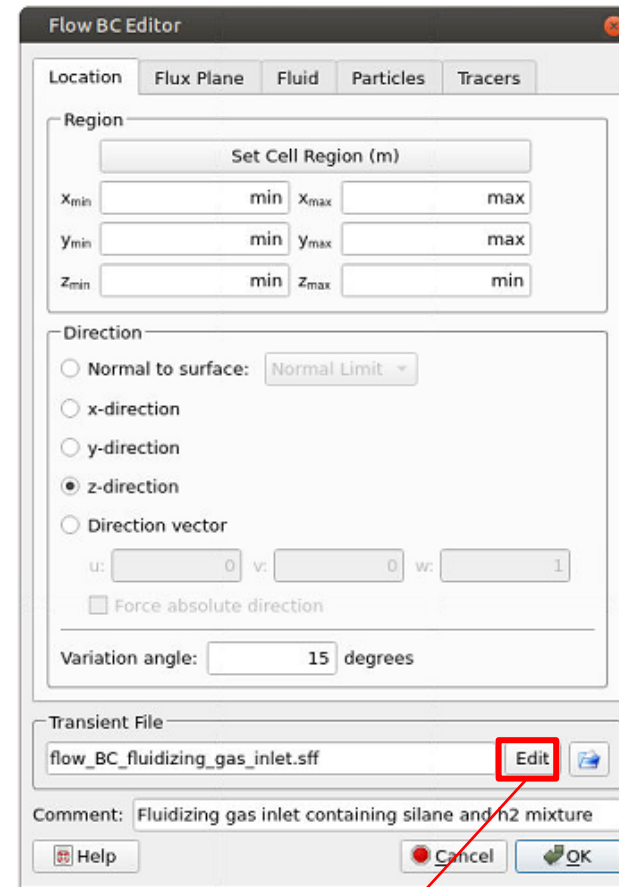
Comment: Top of reactor boundary condition

Buttons: Help, Cancel, OK

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 Editor

Location: Flux Plane | Fluid | Particles | Tracers

Region

Set Cell Region (m)

Xmin: min Xmax: max

Ymin: min Ymax: max

Zmin: min Zmax: min

Direction

☐ Normal to surface: Normal Limit

☐ x-direction

☐ y-direction

☒ z-direction

☐ Direction vector

u: 0 v: 0 w: 1

☐ Force absolute direction

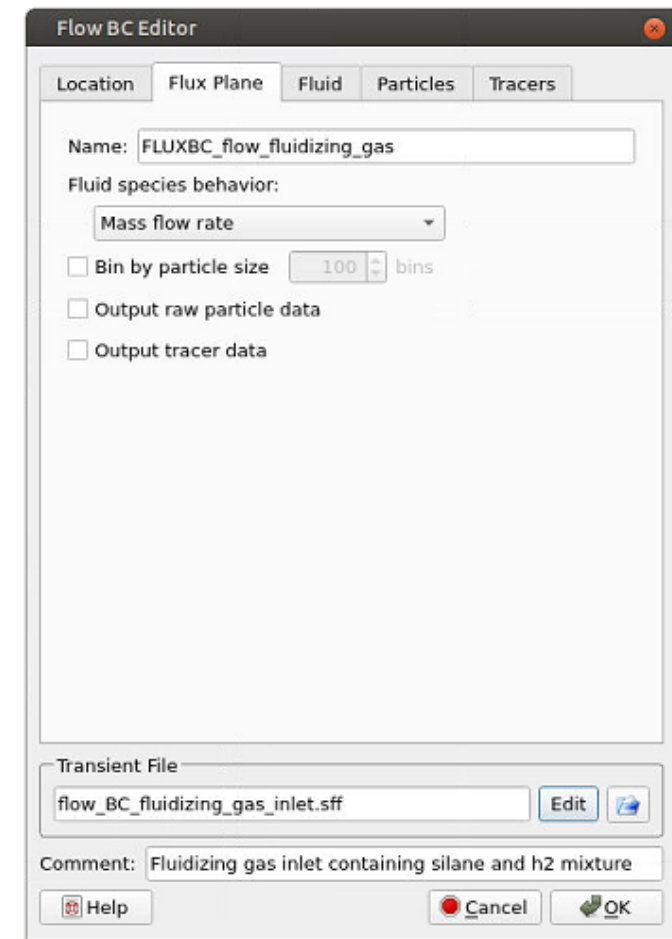
Variation angle: 15 degrees

Transient File

flow_BC_fluidizing_gas_inlet.sff

Comment: Fluidizing gas inlet containing silane and h2 mixture

Buttons: Help, Cancel, OK



Flow BC Editor

Location: Flux Plane | Fluid | Particles | Tracers

Name: FLUXBC_flow_fluidizing_gas

Fluid species behavior:

Mass flow rate

☐ Bin by particle size 100 bins

☐ Output raw particle data

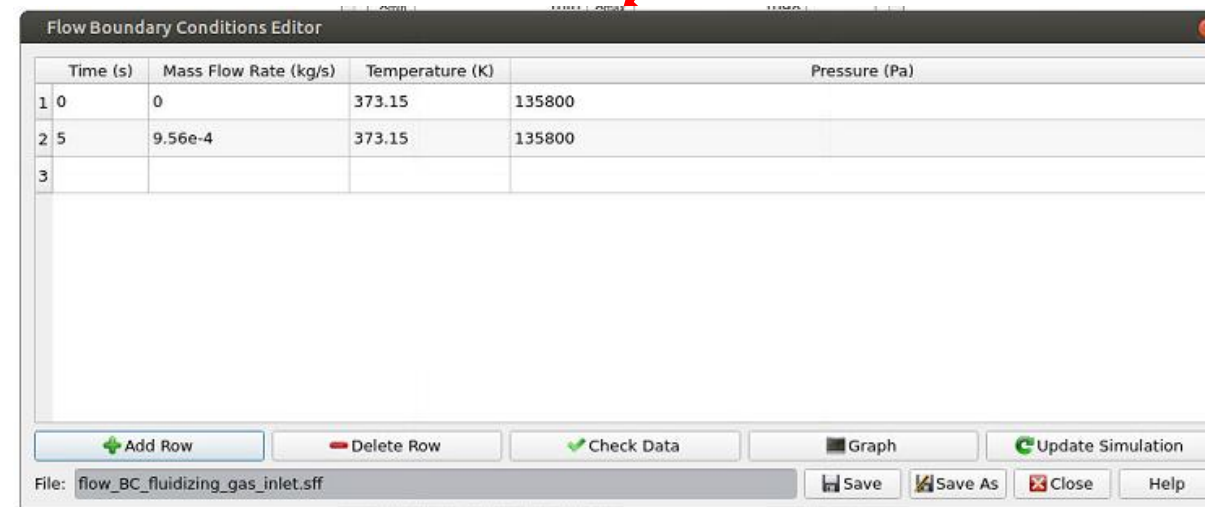
☐ Output tracer data

Transient File

flow_BC_fluidizing_gas_inlet.sff

Comment: Fluidizing gas inlet containing silane and h2 mixture

Buttons: Help, Cancel, OK



Flow Boundary Conditions Editor

	Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	Pressure (Pa)
1	0	0	373.15	135800
2	5	9.56e-4	373.15	135800
3				

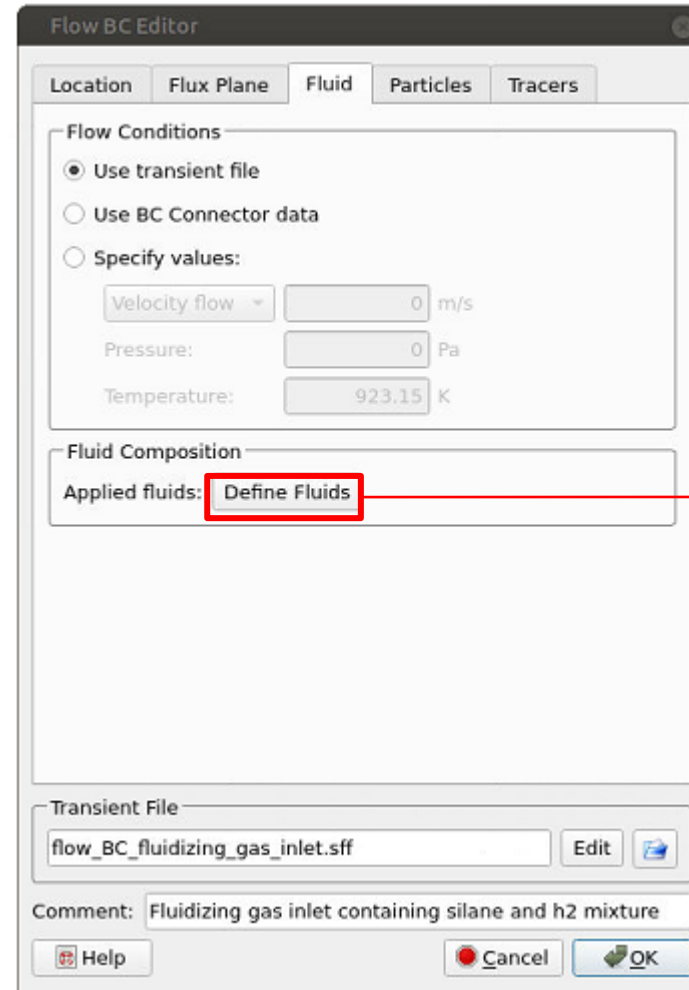
Buttons: Add Row, Delete Row, Check Data, Graph, Update Simulation

File: flow_BC_fluidizing_gas_inlet.sff

Buttons: Save, Save As, Close, Help

Flow BC

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



The Flow BC Editor dialog box has tabs for Location, Flux Plane, Fluid, Particles, and Tracers. The Fluid tab is active. Under Flow Conditions, 'Use transient file' is selected. Under Fluid Composition, 'Applied fluids:' is set to 'Define Fluids'. A red box highlights 'Define Fluids' with an arrow pointing to the Mixture dialog box. The Transient File section shows 'flow_BC_fluidizing_gas_inlet.sff' and a comment 'Fluidizing gas inlet containing silane and h2 mixture'.

Flow BC Editor

Location Flux Plane Fluid Particles Tracers

Flow Conditions

☒ Use transient file
☐ Use BC Connector data
☐ Specify values:

Velocity flow: 0 m/s
Pressure: 0 Pa
Temperature: 923.15 K

Fluid Composition

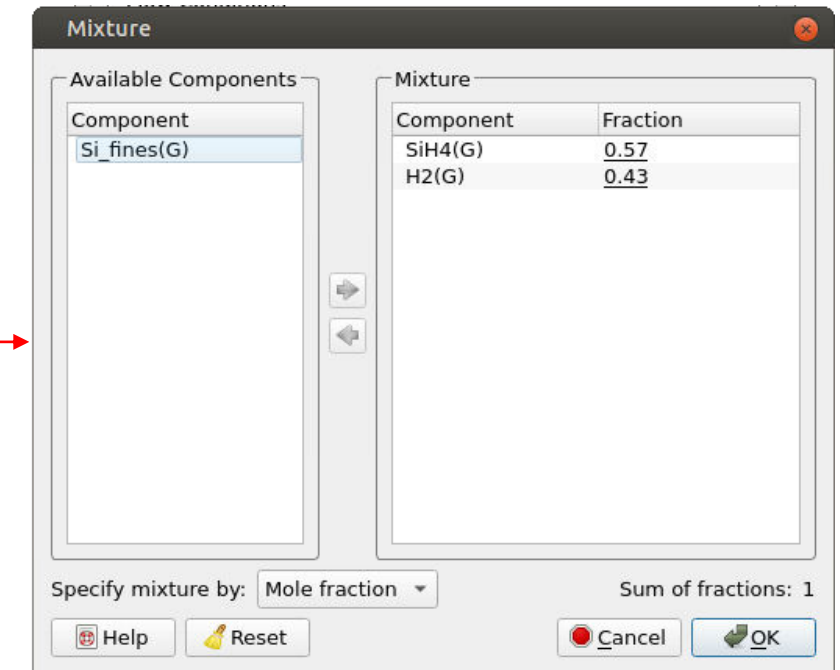
Applied fluids: Define Fluids

Transient File

flow_BC_fluidizing_gas_inlet.sff Edit

Comment: Fluidizing gas inlet containing silane and h2 mixture

Help Cancel OK



The Mixture dialog box shows 'Available Components' with 'Si_fines(G)' selected. The 'Mixture' table lists SiH₄(G) with a fraction of 0.57 and H₂(G) with a fraction of 0.43. The 'Specify mixture by:' dropdown is set to 'Mole fraction' and the 'Sum of fractions' is 1. Buttons for Help, Reset, Cancel, and OK are at the bottom.

Mixture

Available Components

Component
Si_fines(G)

Mixture

Component	Fraction
SiH ₄ (G)	0.57
H ₂ (G)	0.43

Specify mixture by: Mole fraction Sum of fractions: 1

Help Reset Cancel OK

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 ($\frac{m^2}{m^3}$).

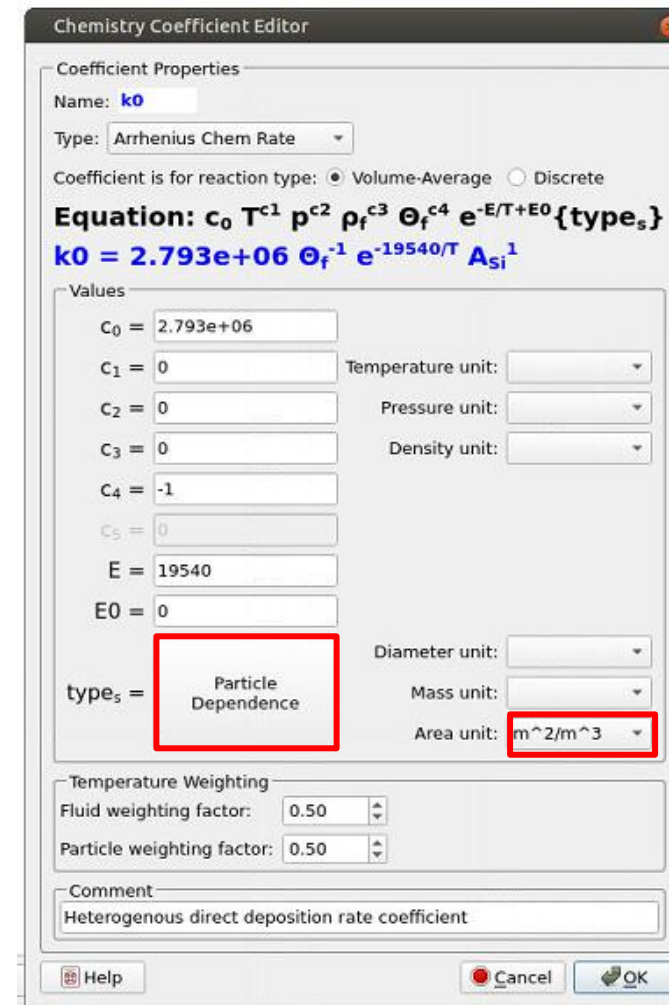
θ_f : fluid volume fraction

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 Coefficient Editor

Coefficient Properties

Name: **k0**

Type: Arrhenius Chem Rate

Coefficient is for reaction type: ☒ Volume-Average ☐ Discrete

Equation: $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \Theta_f^{c_4} e^{-E/T+E0} \{type_s\}$

k0 = 2.793e+06 $\Theta_f^{-1} e^{-19540/T} A_{Si}^1$

Values

C_0 = 2.793e+06

C_1 = 0 Temperature unit:

C_2 = 0 Pressure unit:

C_3 = 0 Density unit:

C_4 = -1

C_5 = 0

E = 19540

E0 = 0

type_s = **Particle Dependence**

Diameter unit:

Mass unit:

Area unit: **m²/m³**

Temperature Weighting

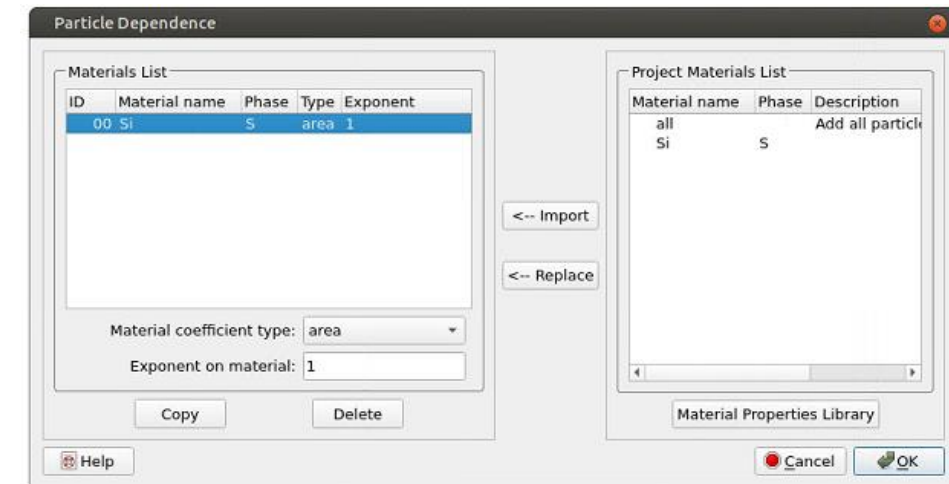
Fluid weighting factor: 0.50

Particle weighting factor: 0.50

Comment

Heterogenous direct deposition rate coefficient

Help Cancel OK



Particle Dependence

Materials List

ID	Material name	Phase	Type	Exponent
00	Si	S	area	1

Material coefficient type: area

Exponent on material: 1

Copy Delete

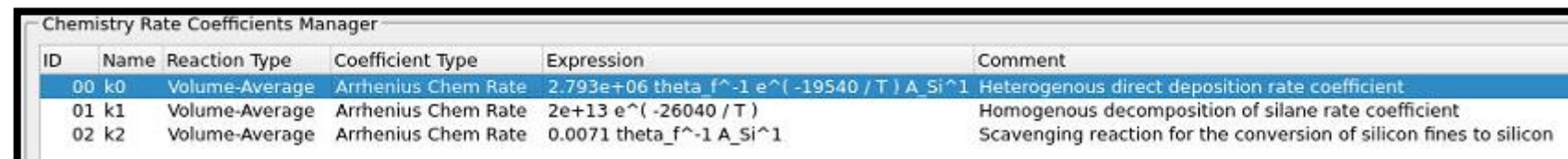
Help

Project Materials List

Material name	Phase	Description
all		Add all particles
Si	S	

Material Properties Library

Cancel OK



Chemistry Rate Coefficients Manager

ID	Name	Reaction Type	Coefficient Type	Expression	Comment
00	k0	Volume-Average	Arrhenius Chem Rate	$2.793e+06 \theta_f^{-1} e^{(-19540/T)} A_{Si}^1$	Heterogenous direct deposition rate coefficient
01	k1	Volume-Average	Arrhenius Chem Rate	$2e+13 e^{(-26040/T)}$	Homogenous decomposition of silane rate coefficient
02	k2	Volume-Average	Arrhenius Chem Rate	$0.0071 \theta_f^{-1} A_{Si}^1$	Scavenging reaction for the conversion of silicon fines to silicon

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	$Si_{fines} \rightarrow Si(s)$	$k_2[Si_{fines}]$

Chemistry Stoichiometric Equation Editor

Stoichiometric Equation Editor

Directions: Choose Equation Units for this Stoichiometric Chemistry. Enter a stoichiometric reaction and rate equation in the blanks provided. Use **Add Material** and **Add Coefficient** to insert either into the equation. Press the **Check** button to verify equation is valid.

Equation Units
Reaction rate units:
Fluid species units:

Enter a stoichiometric reaction:

Expected Power Law rate equation format: $c_0 (k + k - \dots) [material1]^power [material2]^power + c1 \dots$
Example of valid Power Law rate equation format: $1.2 (1.5 * k_0 - 3 * k_1) [H_2O]^{1.5}$
Example of invalid Power Law rate equation format: $(k_0 * k_1) [H_2O]^{1.5}$ Coefficients cannot be multiplied.
Example of LH expected format: $(c_0 k[] + c1 k[] + \dots) / (1 + c2 k[] + c3 k[] + \dots)^power$
Example of groups of rates: $(c_0 k_0 [O_2] - c1 (0.5k_1 - k_2))^{1.5} (c1 k_3) [CO]^{0.5 [O_2]}^{-1}$

Enter a rate equation for the stoichiometric reaction in either Power Law or Langmuir-Hinshelwood form:

Comment

Chemistry Reactions Manager

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: $SiH_4 \Rightarrow Si(S) + 2 H_2$ R00 = $(k_0[SiH_4])$		Direct deposition through heterogeneous reaction
01	VA: Stoichiometric	Equation: $SiH_4 \Rightarrow Si_{fines} + 2 H_2$ R01 = $(k_1[SiH_4])$		Homogeneous decomposition of silane
02	VA: Stoichiometric	Equation: $Si_{fines} \Rightarrow Si(S)$ R02 = $(k_2[Si_{fines}])$		Scavenging reaction for conversion of Silicon fines to Silicon particles

Time Controls

Set Time step and End time

Time Controls

This section allows configuration of the time step size to take during a period of time for the calculation. Only the first row is required. Subsequent rows can be entered to have different time steps for different time periods. For example, starting the calculation at a smaller time step is recommended, and then increasing the time step for rows 2-5 over simulation time.

Time step and duration settings

	Time step		End time	
1.	<input type="text" value="1e-03"/>	s	<input type="text" value="150"/>	s
2.	<input type="text"/>	s	<input type="text"/>	s
3.	<input type="text"/>	s	<input type="text"/>	s
4.	<input type="text"/>	s	<input type="text"/>	s
5.	<input type="text"/>	s	<input type="text"/>	s

[Advanced time step settings](#)

Restart file intervals

Restart interval (IC_###) simulation seconds

Backtrack interval (IC_) realtime minutes

[Help](#)

Visualization Data Output

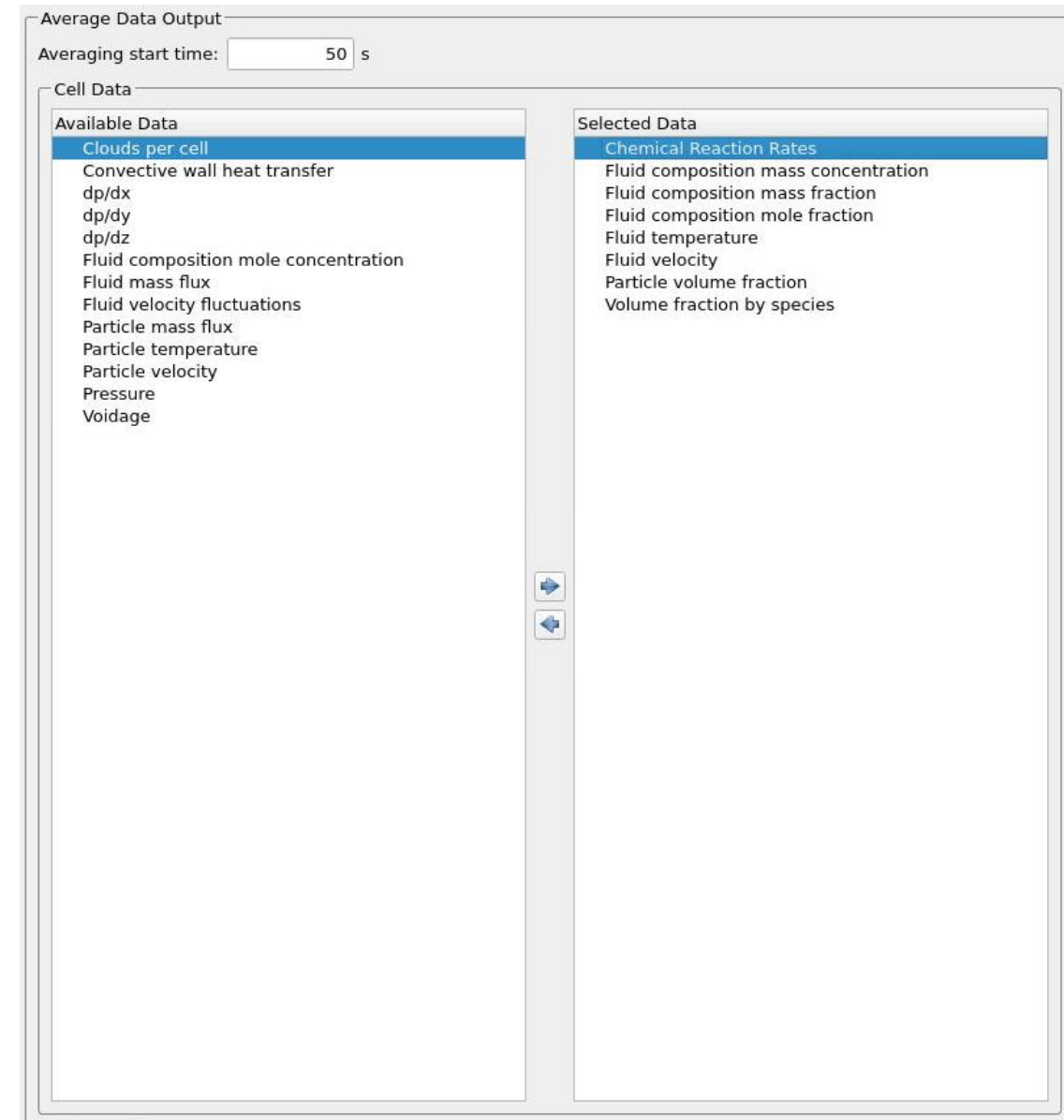
Set Output file interval and select the options shown for Visualization Data Output.

The screenshot shows the 'Visualization Data Output' dialog box. It is divided into several sections:

- Output file format:** Two radio buttons are present: 'Tecplot (*.plt files)' (which is selected) and 'GMV (Gmv.* files)'.
- Output file interval:** Two radio buttons are present: 'Constant' (selected) and 'Time-varying'. The 'Constant' section includes a text box with the value '1', followed by 's', and labels for 'End time: 150s' and 'Number of output files: 151'. The 'Time-varying' section has an empty text box and an 'Edit' button.
- Cell Data:** A list of 'Available Data' on the left and a list of 'Selected Data' on the right. The 'Available Data' list includes: Cell ID, Clouds per cell, Convective wall heat transfer, dp/dx, dp/dy, Dynamic pressure, Fluid composition mass concentration, Fluid composition mole concentration, Fluid mass flux, P1 incident radiation flux, P1 radiation flux, P1 radiation flux from walls, P1 radiation to fluids, P1 radiation to particles, Particle mass flux, Particle temperature, and Particle velocity. The 'Selected Data' list includes: Bulk density, Cell indices, Cell volume, CFL, Chemical Reaction Rates, dp/dz, Fluid composition mass fraction, Fluid composition mole fraction, Fluid density, Fluid temperature, Fluid velocity, Particle volume fraction, and Pressure.
- Particle Data:** A list of 'Available Data' on the left and a list of 'Selected Data' on the right. The 'Available Data' list includes: Cell ID, Drag, Liquid fraction total, Liquid mass total, P1 radiation flux, Particle material, Particle velocity, Particles per cloud, Residence time, and Species. The 'Selected Data' list includes: Chemical Reaction Rates, Cloud ID, Cloud mass, Particle density, Particle mass, Particle size, Particle speed, Particle temperature, and Particle volume fraction.

Average Data Output

Select the following outputs under the
Average Data window

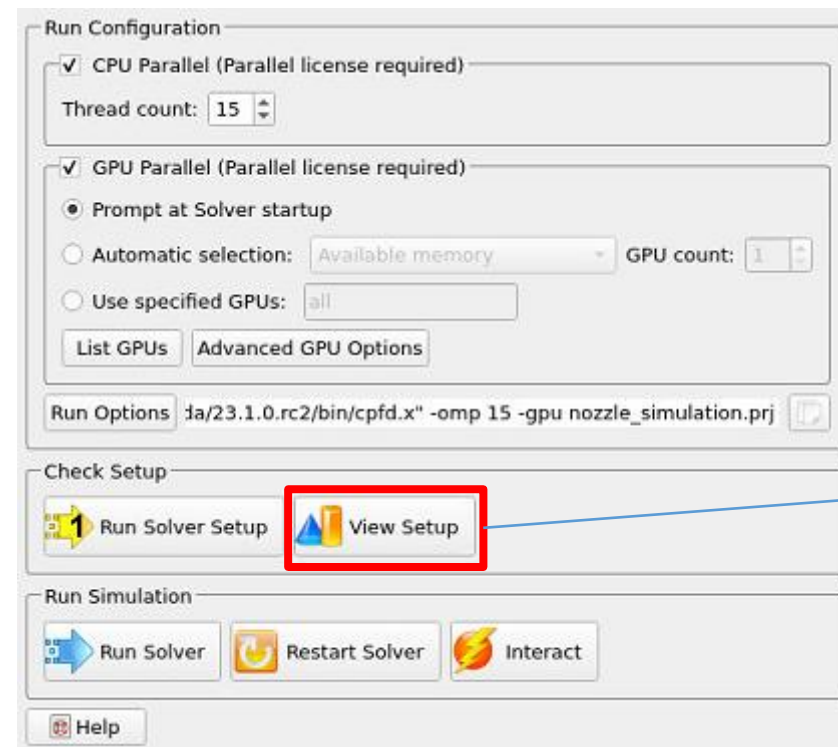


Run

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

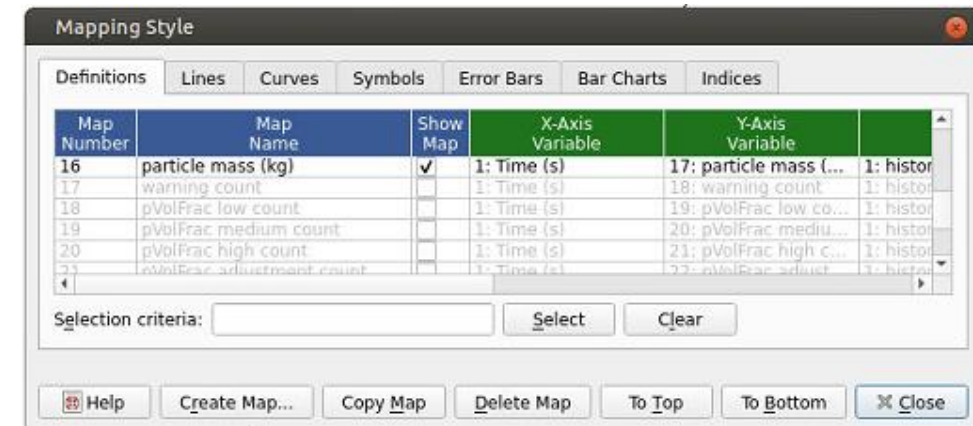
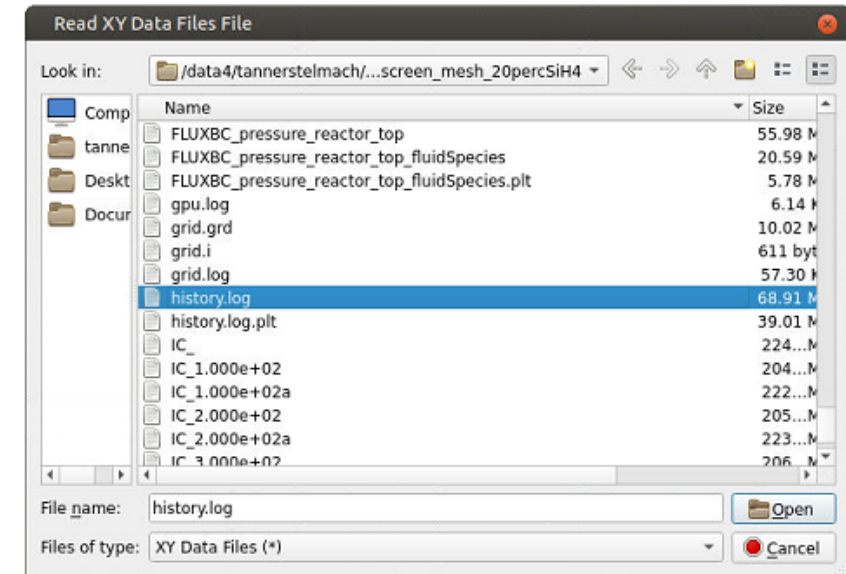


Post-Processing: Silicon Deposition Rate

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*

Specify Equations

Equation(s)

{Time (hr)} = {Time (s)}/3600

Data Set Info... ☒ Ignore divide by zero errors Save Equations... Load Equations...

Default Equation Modifiers

Zones to Alter

1: history.log (/data4/tannerstelmach/sil)

All Active None

Index Ranges

	Start	End	Skip
I-Index	1	Mx	1
J-Index	1	Mx	1
K-Index	1	Mx	1

New var data type: Auto

New var location: Auto

Help Compute Close

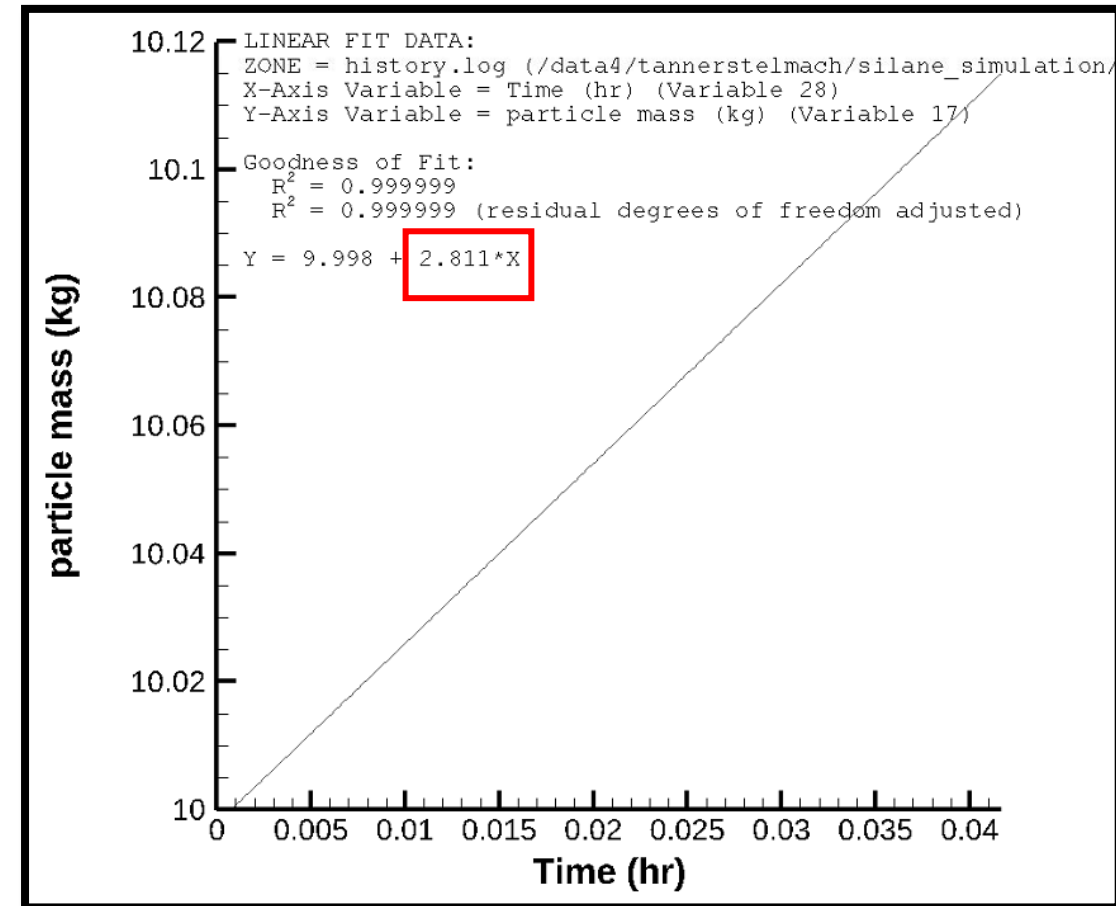
Post-Processing: Silicon Deposition Rate

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



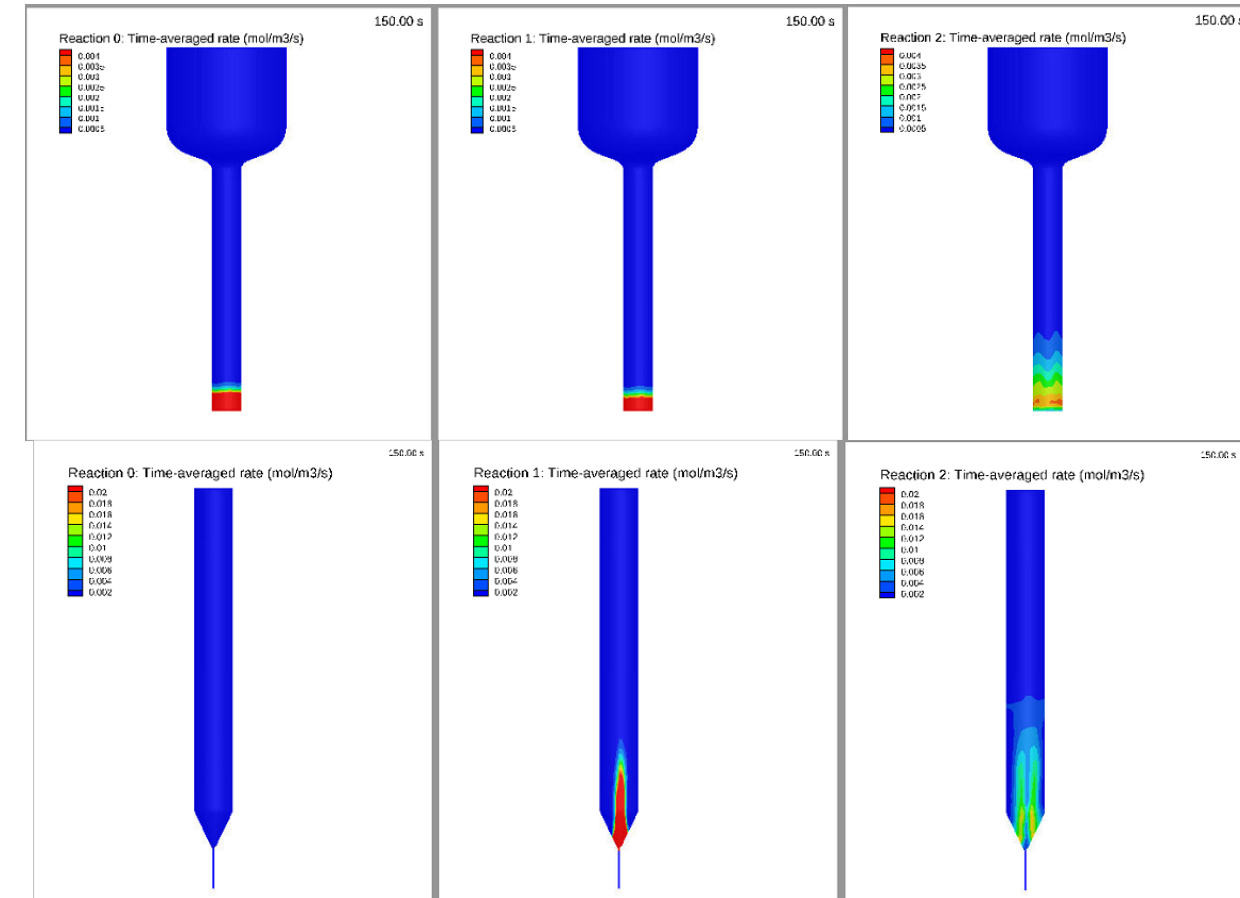
Post-Processing: Reaction Rate Output

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/>

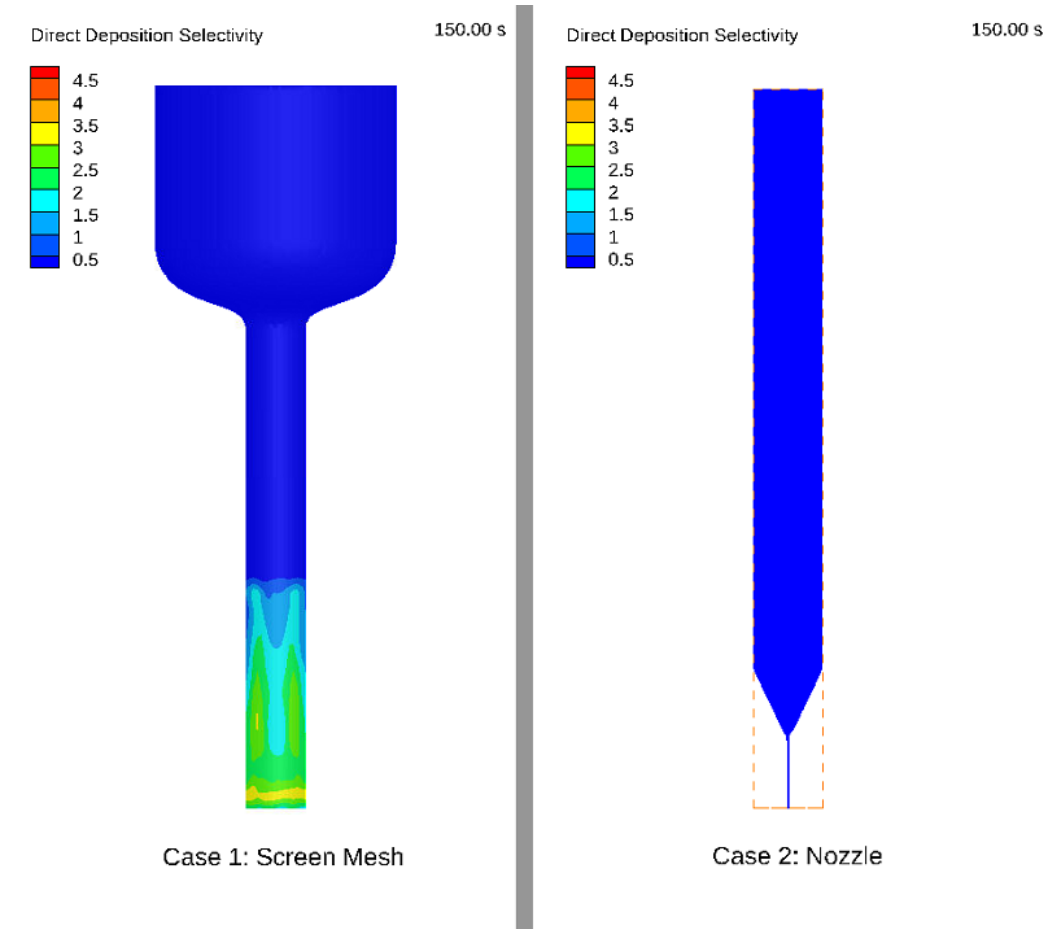


Post-Processing: Direct Deposition Reaction Selectivity

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*

Specify Equations

Equation(s)

{Direct Deposition Selectivity} = {Time-averaged rate of volume-average stoichiometric reaction 00}/{Time-averaged rate of volume-average stoichiometric reaction 01}

Data Set Info... ☒ Ignore divide by zero errors Save Equations... Load Equations...

Default Equation Modifiers

Zones to Alter

- 1: Cells
- 2: Particles
- 3: 2010-07-08_silane_reactor_cone_inlet
- 4: Flow BC (000)
- 5: Pressure BC (000)

All Active None

Index Ranges

	Start	End	Skip
I-Index	1	Mx	1
J-Index	1	Mx	1
K-Index	1	Mx	1

New var data type: Auto

New var location: Auto

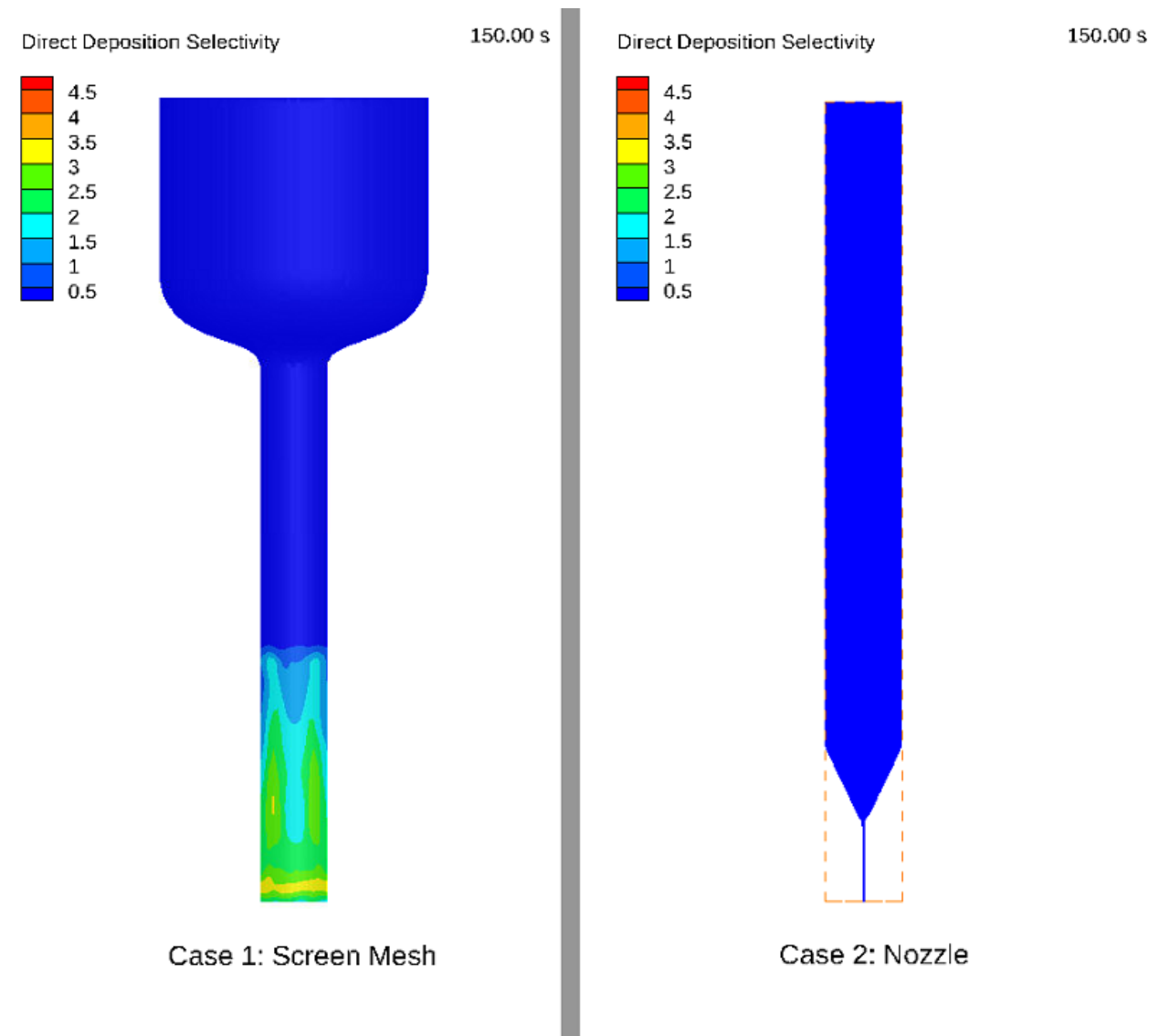
Help Compute Close

Create a slice and select the appropriate data

Double click the contour bar and select the variable that we just created (*Direct Deposition Selectivity*).

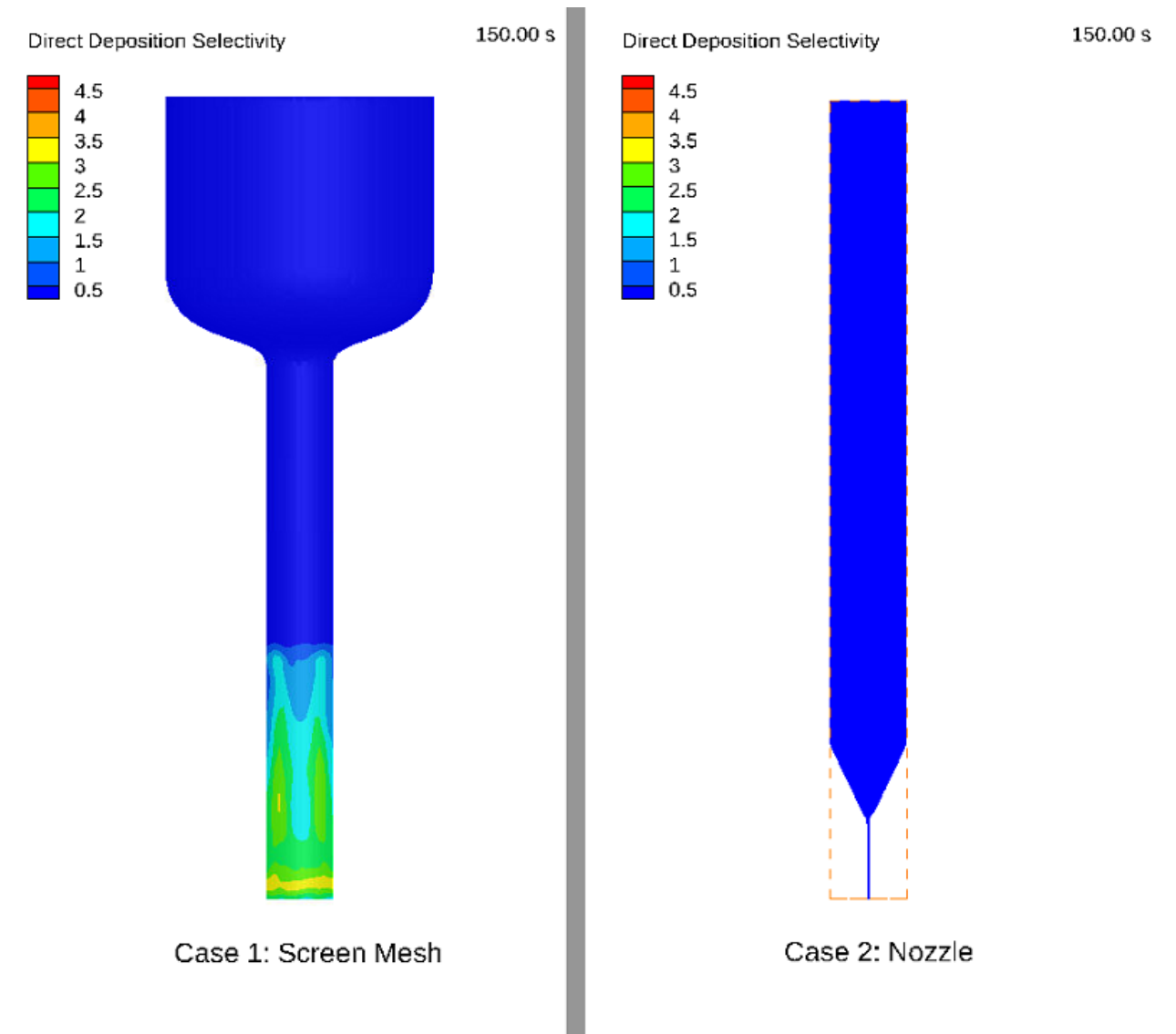
Adjust the color bar to the desired view. Here we use *Modified Rainbow (less green)*

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

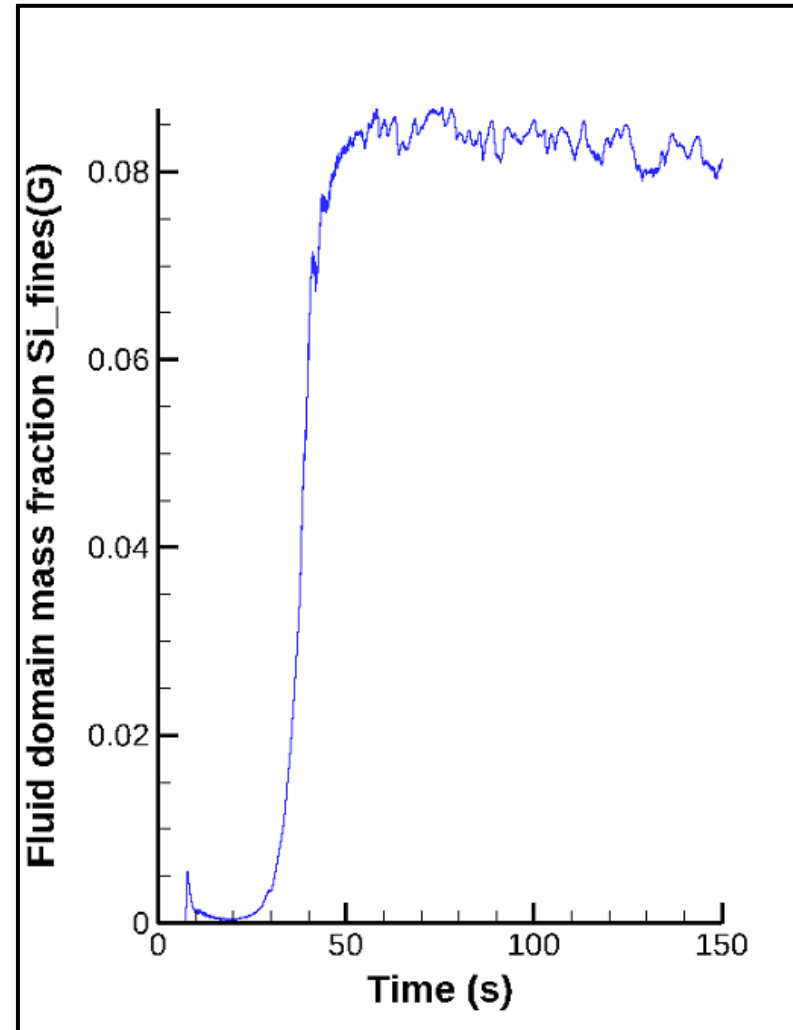
We would like to create a plot of the time-averaged mass fraction of silicon fines at the reactor exit.

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

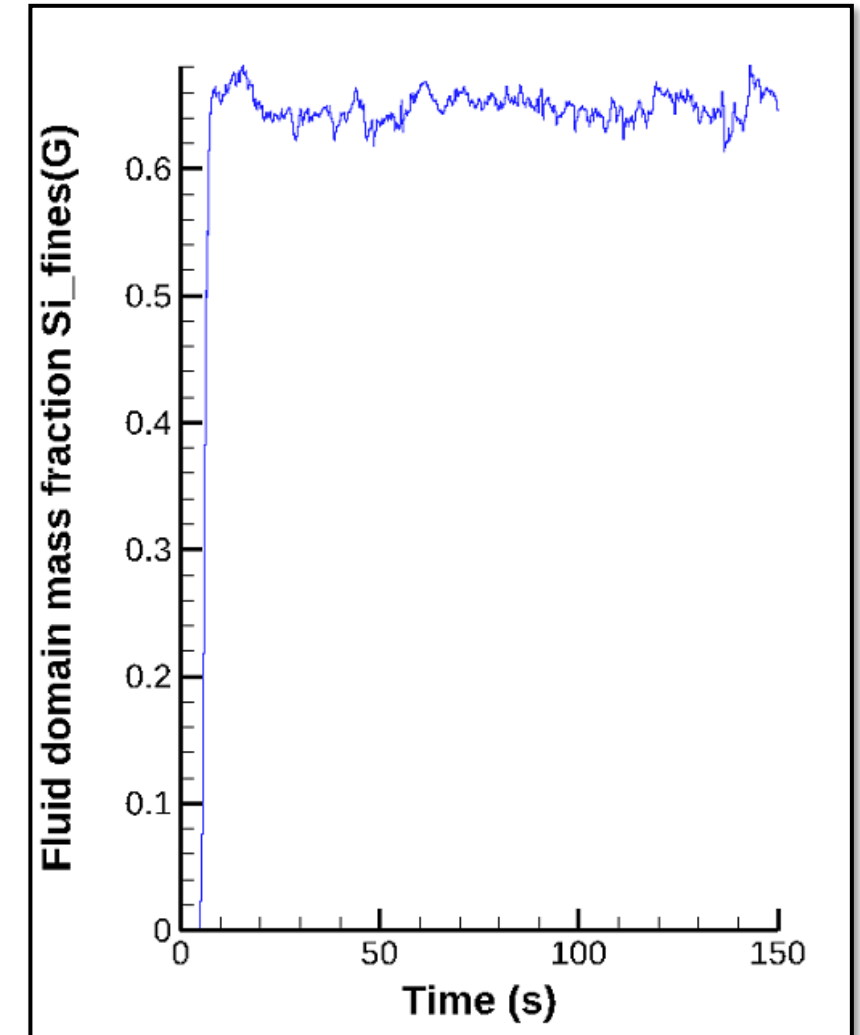
Post-Processing: Silicon Fines Exit Mass Fraction

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 SiH_4 (mol%)	Flowrate (kg/s)
20%	4.0e-04
50%	8.5e-04
80%	1.3e-03

Flow Boundary Conditions Editor

	Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	
1	0	0	373.15	135800
2	5	4.0e-4	373.15	135800
3				

+ Add Row

- Delete Row

✓ Check Data

■ Graph

↻ Update Simulation

File: flow_BC_fluidizing_gas_inlet.sff

Save

Save As

Close

Help

Mixture

Available Components

Component

Si_fines(G)

Mixture

Component	Fraction
H2(G)	0.8
SiH4(G)	0.2

Specify mixture by: Mole fraction

Sum of fractions: 1

Help

Reset

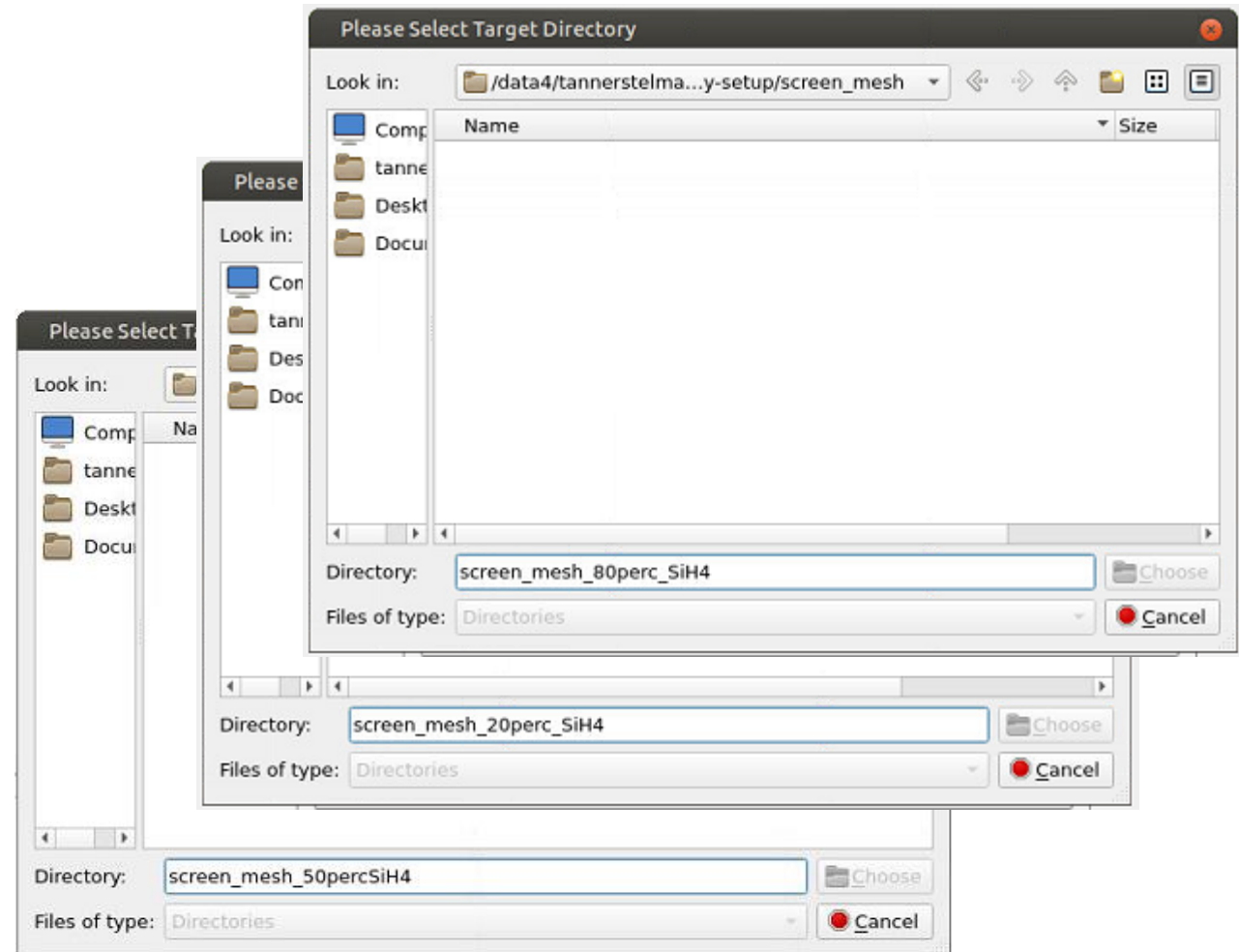
Cancel

OK

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

