

# Silane Deposition: Setup and Analysis

CPFD Software

[www.cpfd-software.com](http://www.cpfd-software.com)

# Silane Deposition

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

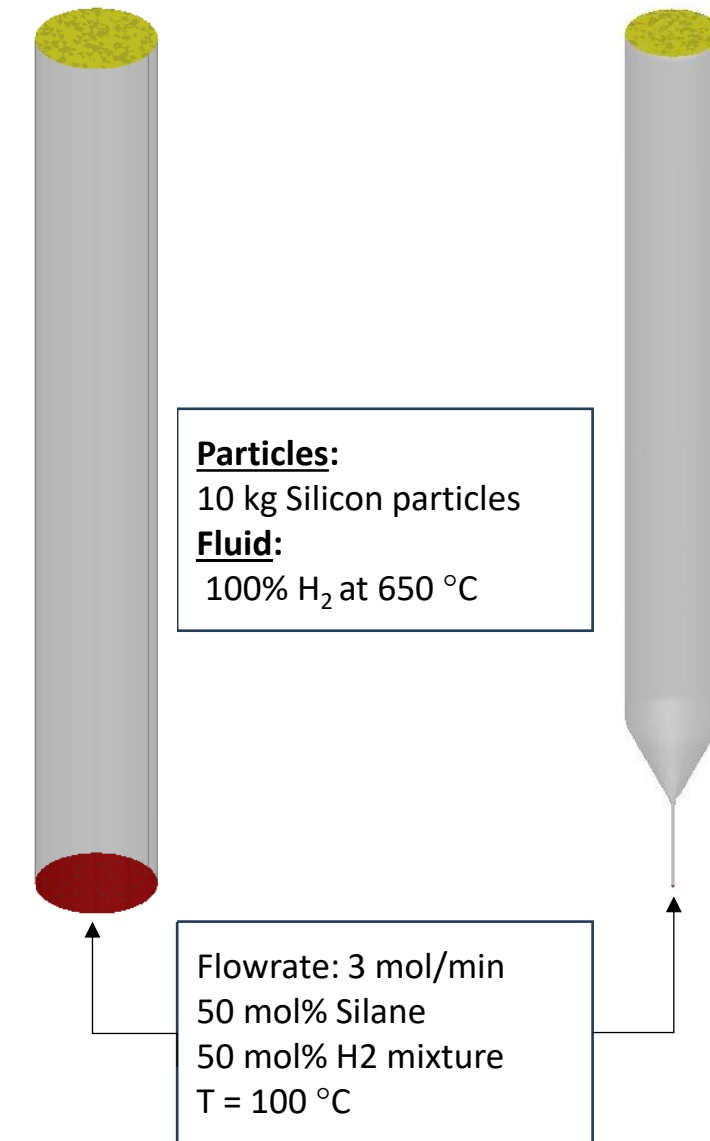
Case 1: Screen Mesh

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

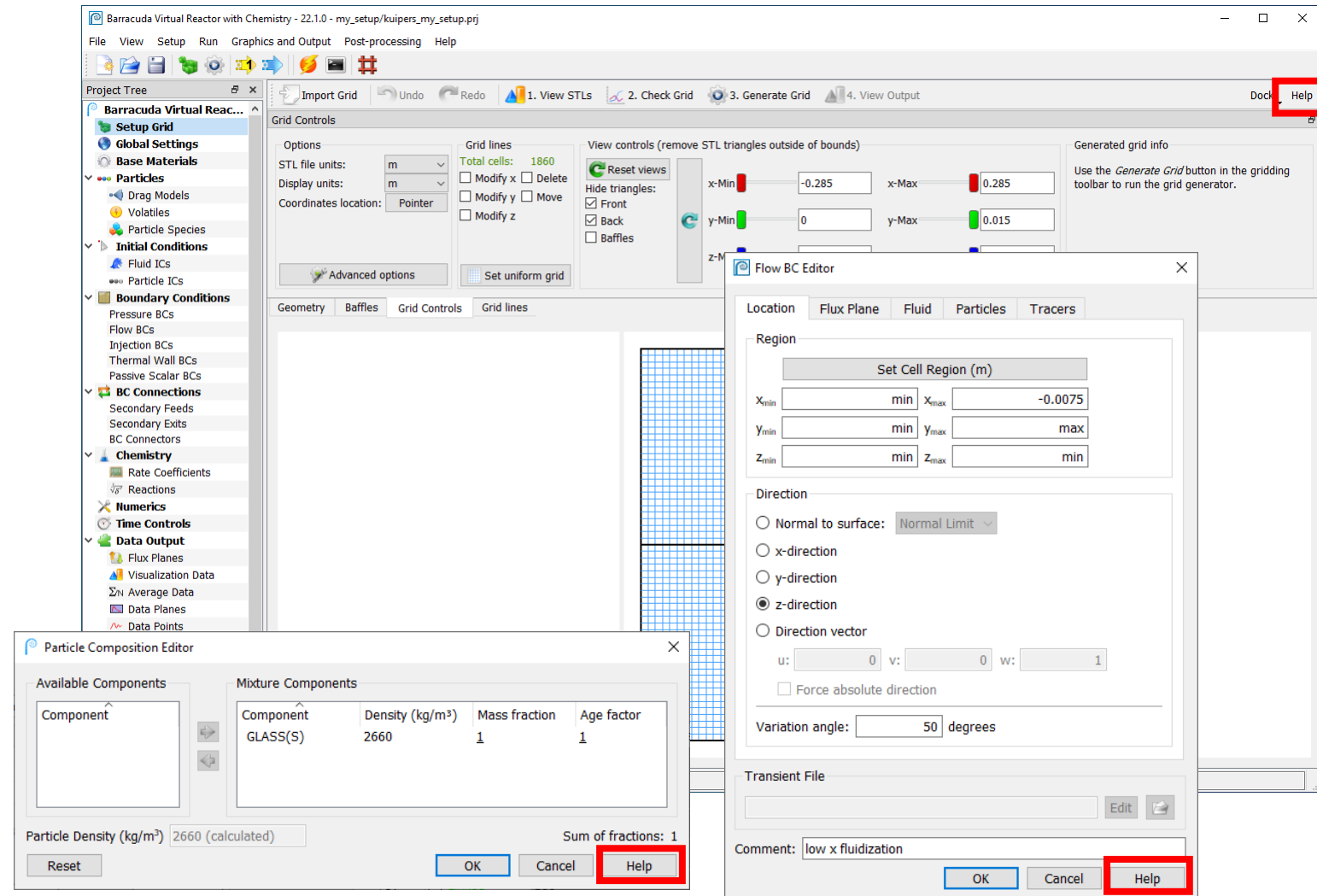
System Pressure: 1.358 bar



# 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.



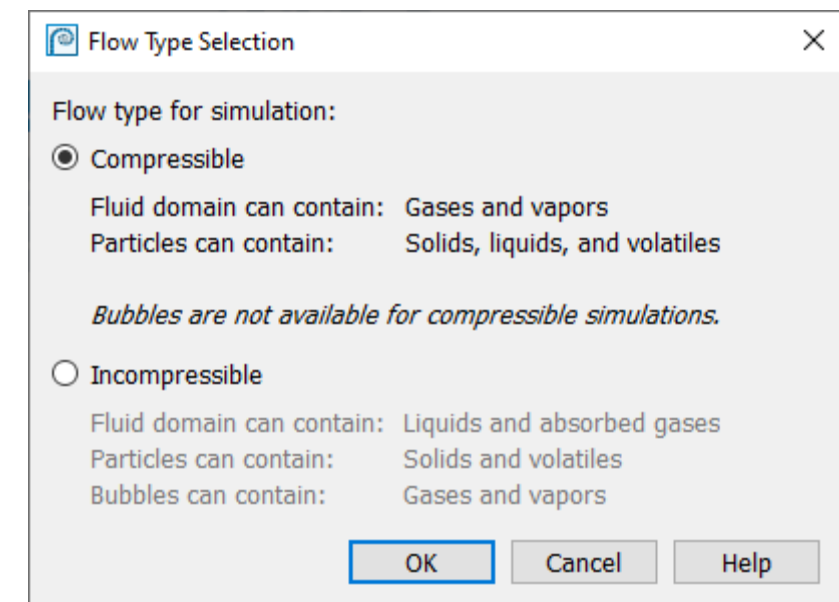
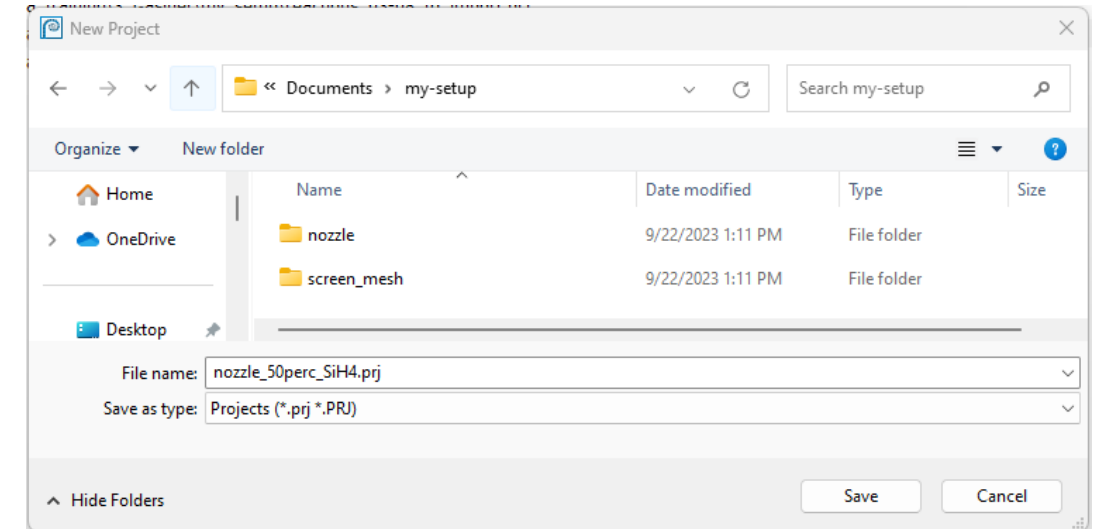
# Project File

We will demonstrate how to run the project with the case of 57% mole fraction SiH<sub>4</sub> for each reactor geometry. Locate the following directories:

- my-setup\nozzle\57perc\_SiH<sub>4</sub>
- my-setup\screen\_mesh\57perc\_SiH<sub>4</sub>

Use the following project names:

- nozzle\_57percSiH<sub>4</sub>.prj
- screen\_mesh\_57percSiH<sub>4</sub>.prj



# Screen Mesh: Setup Grid

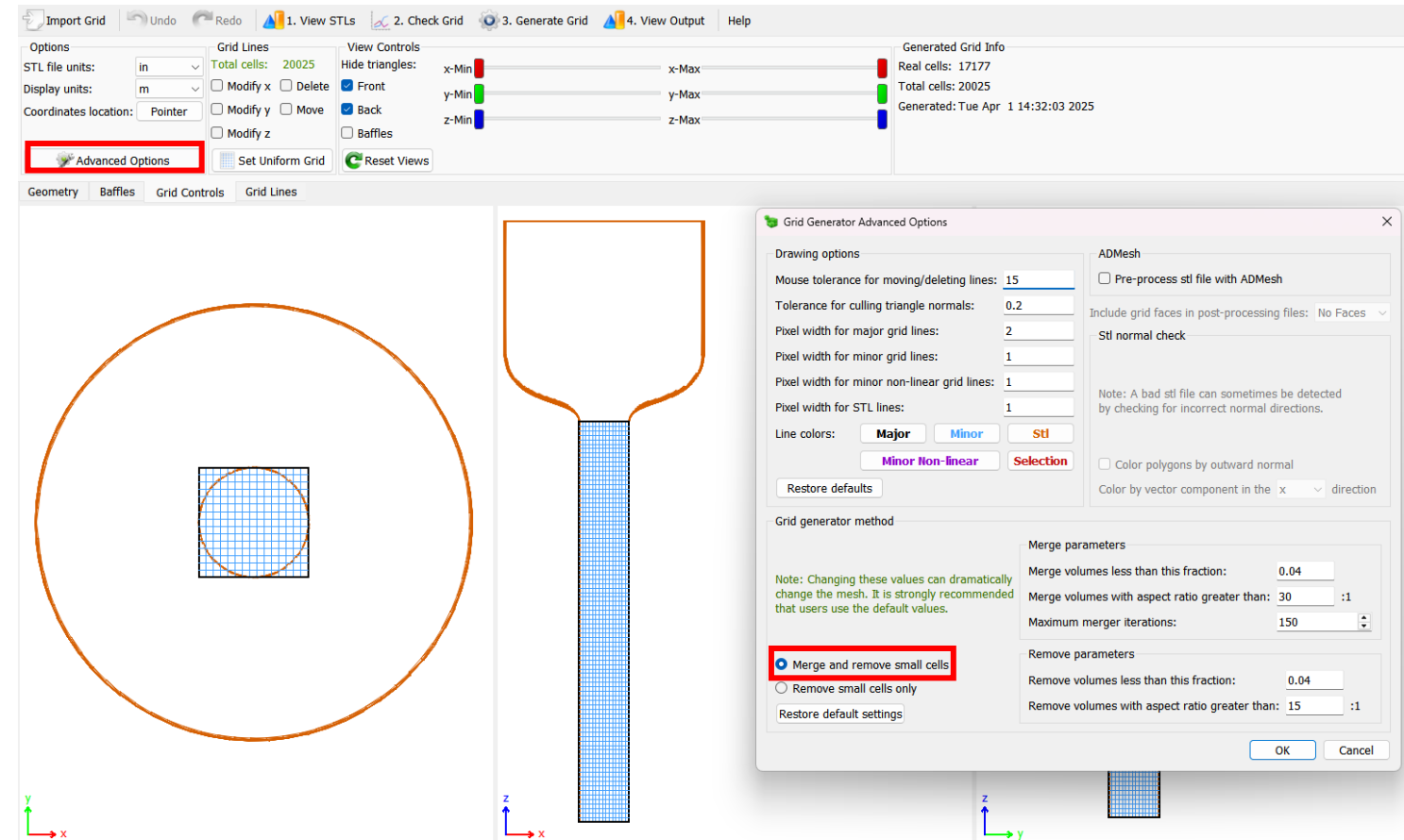
In the  
screen\_mesh/screen\_mesh\_57perc\_  
SiH4.prj file

## Geometry tab:

- Add 2010-07-02\_silane\_reactor\_flat\_inlet.stl

## Controls tab:

- Set STL file units to inches
- Under the Advanced options, use Merge and remove small cells



# Nozzle: Setup Grid

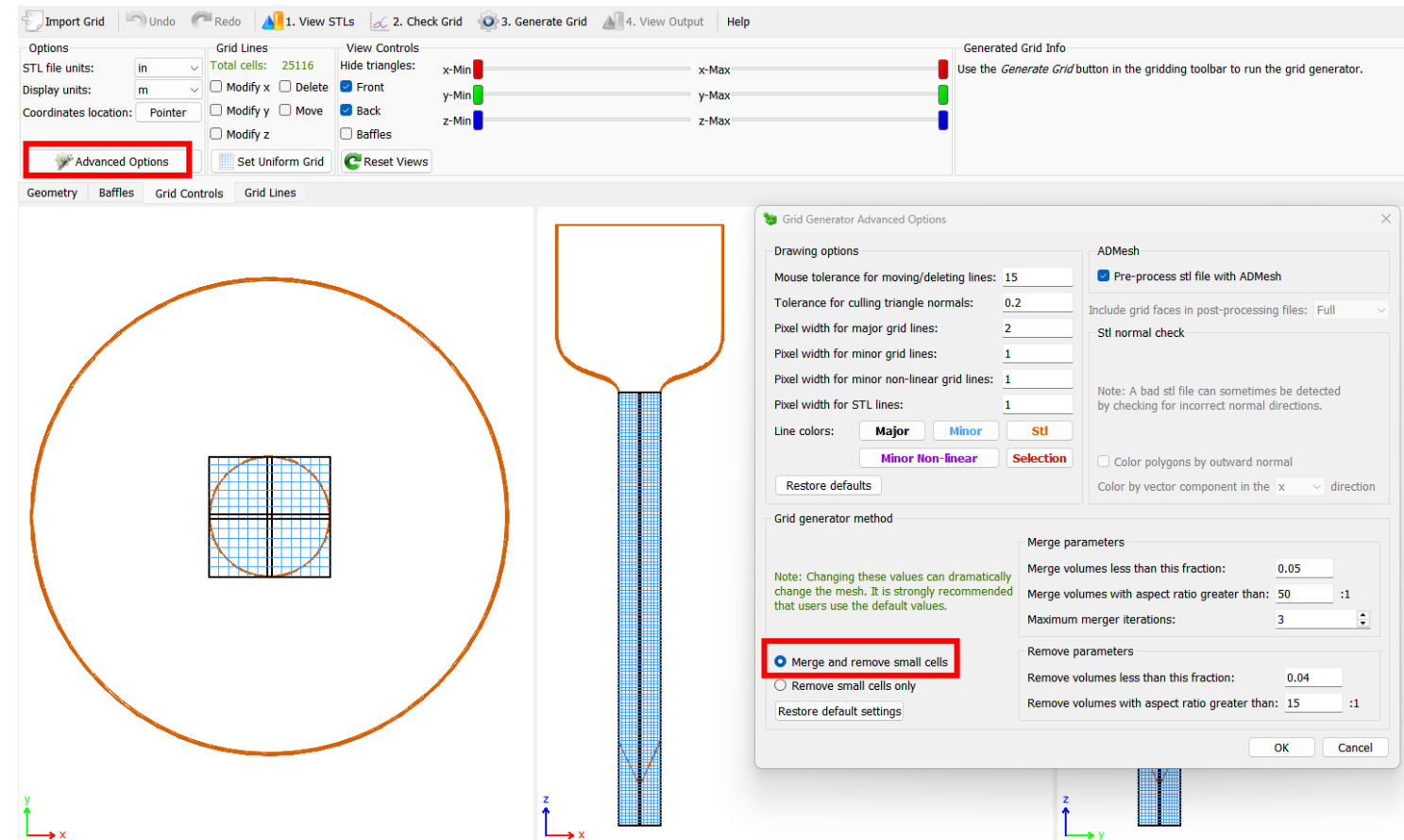
In the nozzle/nozzle\_57perc\_SiH4.prj file

## Geometry tab:

- Add 2010-07-02\_silane\_reactor\_cone.stl

## Controls tab:

- Set STL file units to inches
- Under the Advanced options, use Merge and remove small cells



# Global Settings

Set Gravity in the z-direction

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

Select Enable particle-particle heat conduction setting

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

☒ Use specified values: x-direction:  m/s<sup>2</sup> y-direction:  m/s<sup>2</sup> z-direction:  m/s<sup>2</sup>

☐ Rotate about major axis:  Rotation velocity:  rad/s

☐ Use transient file:   

Thermal Settings

☐ Isothermal  
Temperature:  K

☒ Thermal

Convection

Conduction  
☒ Enable particle-to-particle heat conduction

Radiation  
☒ 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

# Base Materials

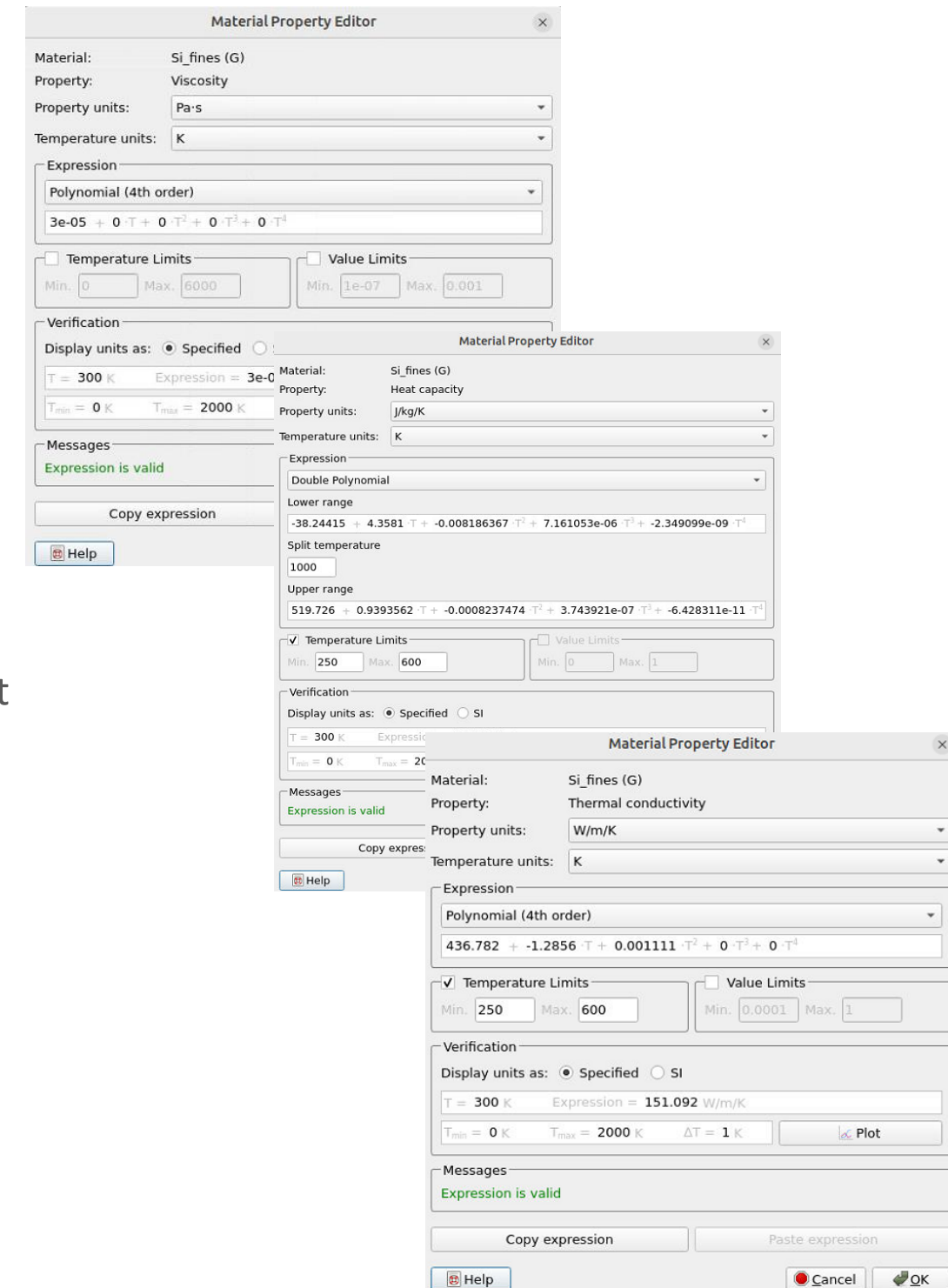
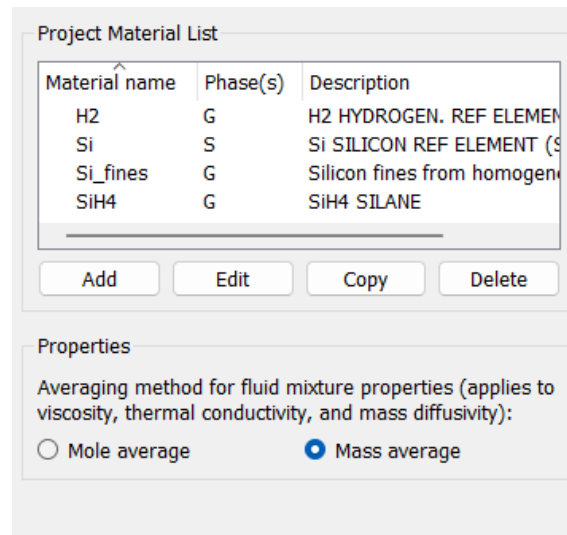
## Import H2, Si(S), and SiH4

### Add Si\_fines (Silicon fines)

- Create a copy of Silicon base material and label it “Si\_fines”
- Change the phase to “Gas”
  - Note that gas is chosen here due to the reaction chemistry. Barracuda does not have the functionality for deposition without a seed particle
- MW = 28.0855 g/mol
- Viscosity =  $3\text{e-}5 \text{ Pa}\cdot\text{s}$
- The same heat capacity and thermal conductivity values are used from the Silicon base material.

### In order to have the chemical equations balanced use the following molecular weights:

- 28.0855 g/mol for both Silicon and Silicon\_fines
- 32.1171 g/mol for SiH4





# Particles

Set Close pack volume fraction: 0.54

Normal-to-wall momentum retention: 0.3

Tangent-to-wall momentum retention: 0.99

Particles

Contact and Collision Models

Close pack volume fraction:

Momentum redirection model:

Maximum momentum redirection from collision:

☐ Blended acceleration model for the contact force

☒ Transfer liquid mass on collision

Wall Interactions

Normal-to-wall momentum retention:

Tangent-to-wall momentum retention:

Diffuse bounce:

Cloud Options

Global cloud resolution:

☒ Automatic:

☐ Specify resolution:

☐ Allow clouds to represent fractional particles

Dense Fluid Forces

☐ Enable virtual mass force

☐ Enable lift force

# 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 Particles	Si	75 to 425 micron-diameter	1	1	WenYu-Ergun	Off

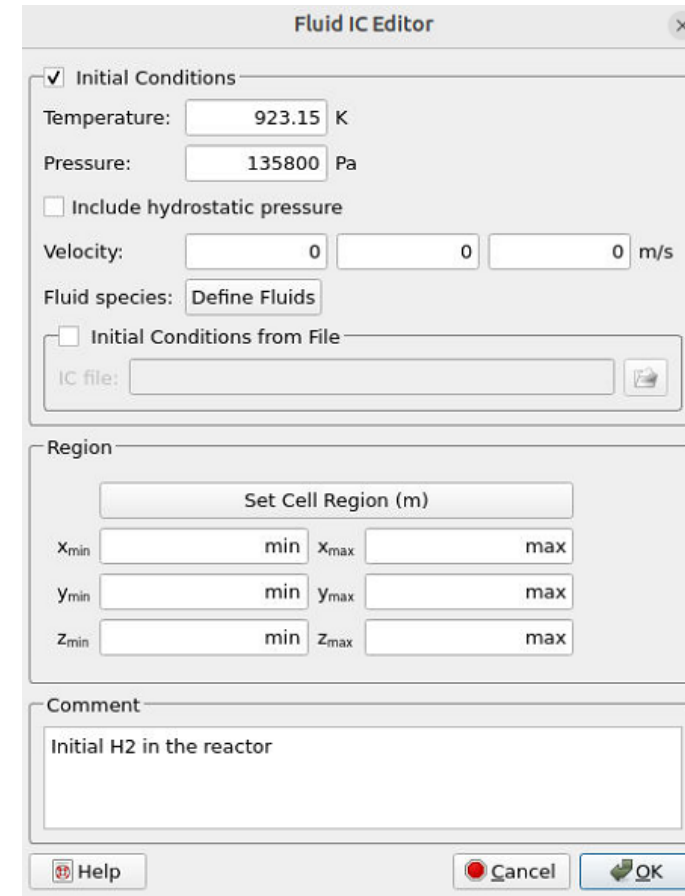
# Screen Mesh: Fluid and Particle ICs

## Fluid IC

- Pressure = 135800 Pa
- Fluid species = 100% H<sub>2</sub>

## Particle IC

- Initialize mass in region
- Species = Silicon (S)
- Mass = 10 kg
- Set region
  - 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

☐ Include hydrostatic pressure

Velocity: 0 0 0 m/s

Fluid species: Define Fluids

☐ Initial Conditions from File

IC file:

Region

Set Cell Region (m)

X<sub>min</sub> min X<sub>max</sub> max

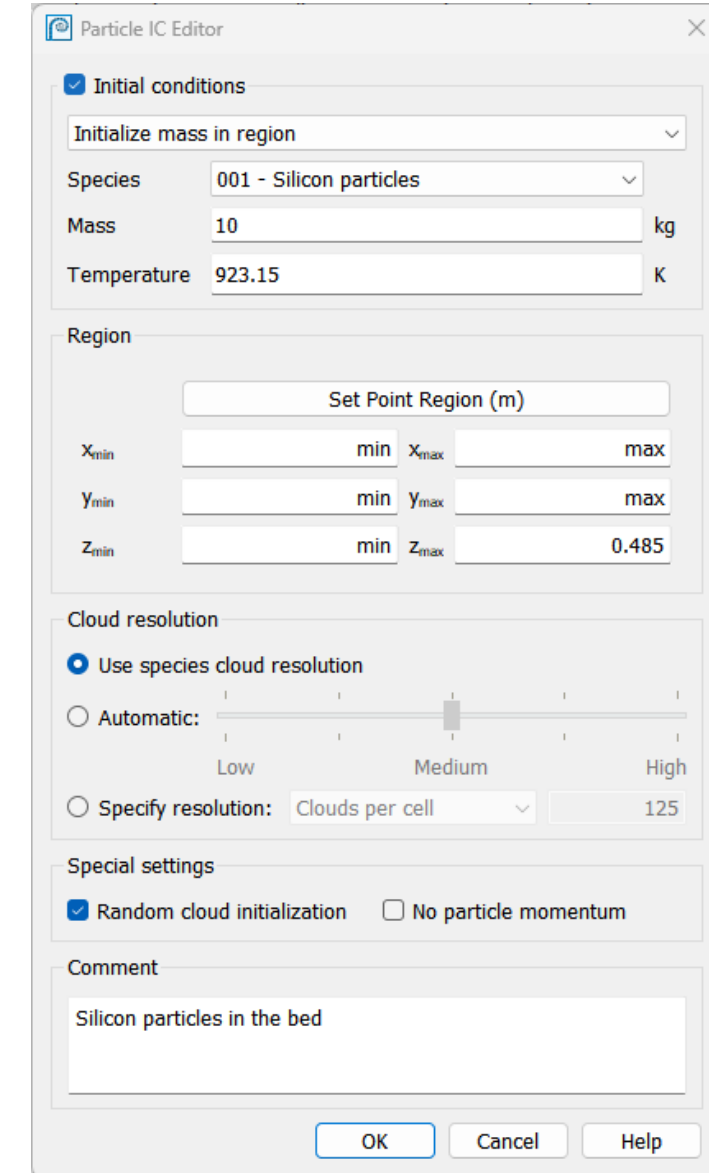
Y<sub>min</sub> min Y<sub>max</sub> max

Z<sub>min</sub> min Z<sub>max</sub> max

Comment

Initial H<sub>2</sub> 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<sub>min</sub> min X<sub>max</sub> max

Y<sub>min</sub> min Y<sub>max</sub> max

Z<sub>min</sub> min Z<sub>max</sub> 0.485

Cloud resolution

☒ Use species cloud resolution

☐ Automatic: Low Medium High

☐ Specify resolution: Clouds per cell 125

Special settings

☒ Random cloud initialization ☐ No particle momentum

Comment

Silicon particles in the bed

OK Cancel Help

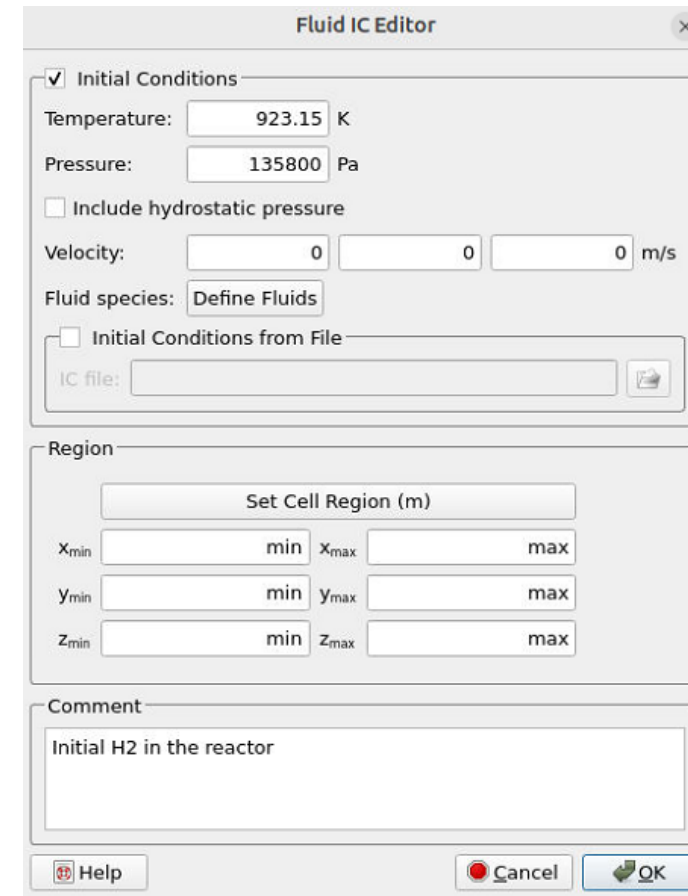
# Nozzle: Fluid and Particle ICs

## Fluid IC

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

## Particle IC

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



Fluid IC Editor

☒ Initial Conditions

Temperature: 923.15 K

Pressure: 135800 Pa

☐ Include hydrostatic pressure

Velocity: 0 0 0 m/s

Fluid species: Define Fluids

☐ Initial Conditions from File

IC file:

Region

Set Cell Region (m)

x<sub>min</sub> min x<sub>max</sub> max

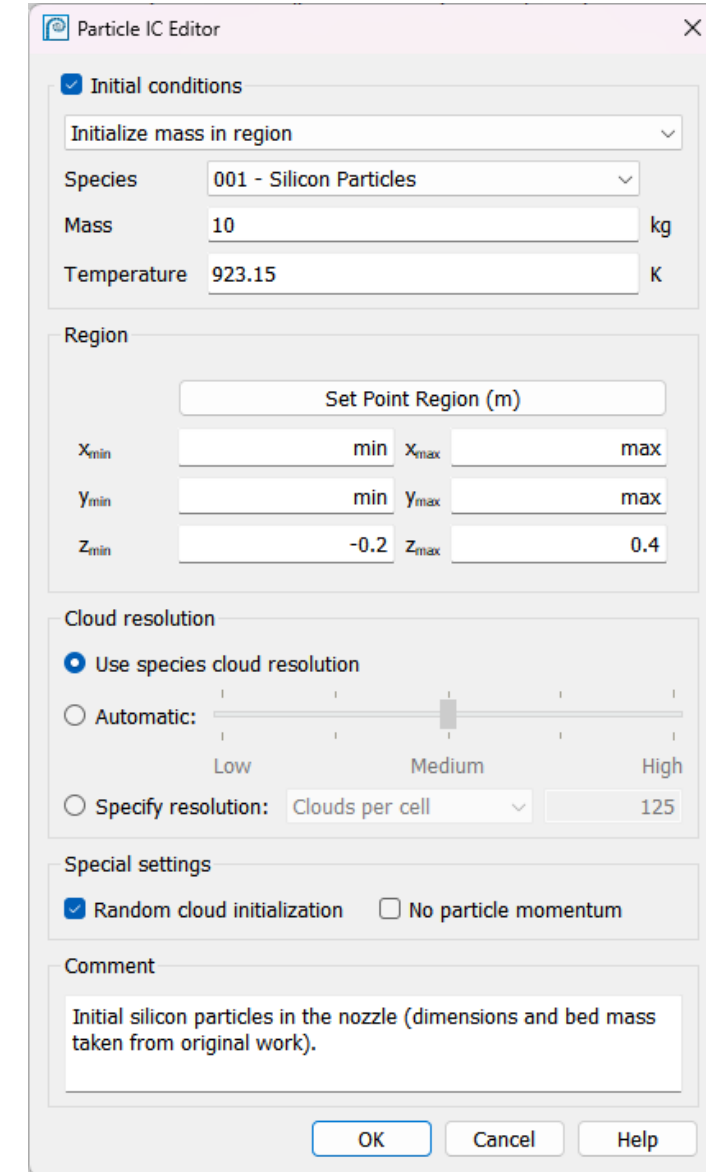
y<sub>min</sub> min y<sub>max</sub> max

z<sub>min</sub> min z<sub>max</sub> 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<sub>min</sub> min x<sub>max</sub> max

y<sub>min</sub> min y<sub>max</sub> max

z<sub>min</sub> -0.2 z<sub>max</sub> 0.4

Cloud resolution

☒ Use species cloud resolution

☐ Automatic:  Low Medium High

☐ Specify resolution: Clouds per cell 125

Special settings

☒ Random cloud initialization ☐ No particle momentum

Comment

Initial silicon particles in the nozzle (dimensions and bed mass taken from original work).

OK Cancel Help

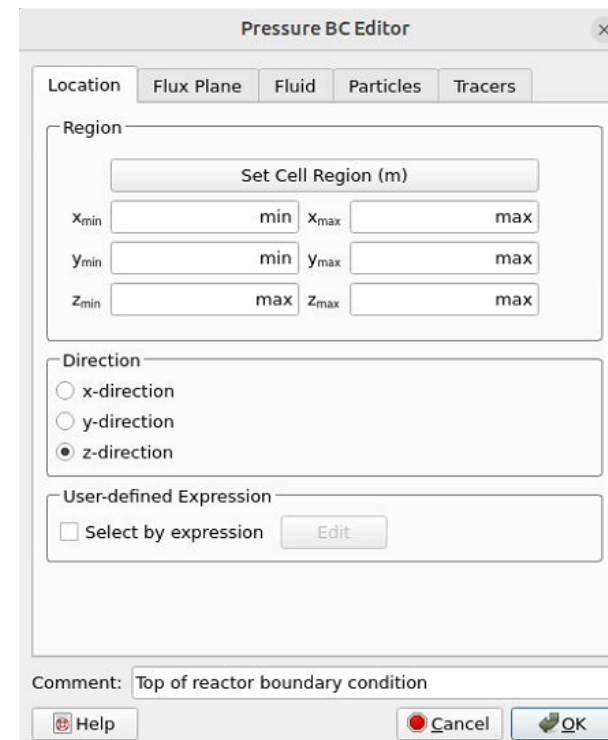
# Pressure BC

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

In the fluid pane, select 100% H<sub>2</sub>

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

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



Pressure BC Editor

Location: Flux Plane | Fluid | Particles | Tracers

Region

Set Cell Region (m)

Xmin: min Xmax: max

Ymin: min Ymax: max

Zmin: max Zmax: max

Direction

☐ x-direction

☐ y-direction

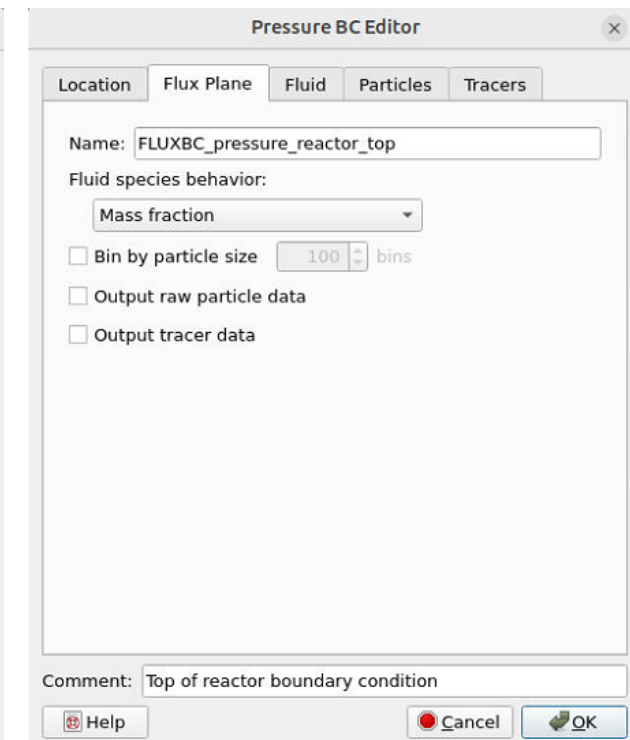
☒ z-direction

User-defined Expression

☐ Select by expression Edit

Comment: Top of reactor boundary condition

Help Cancel OK



Pressure BC Editor

Location: Flux Plane | Fluid | Particles | Tracers

Name: FLUXBC\_pressure\_reactor\_top

Fluid species behavior:

Mass fraction

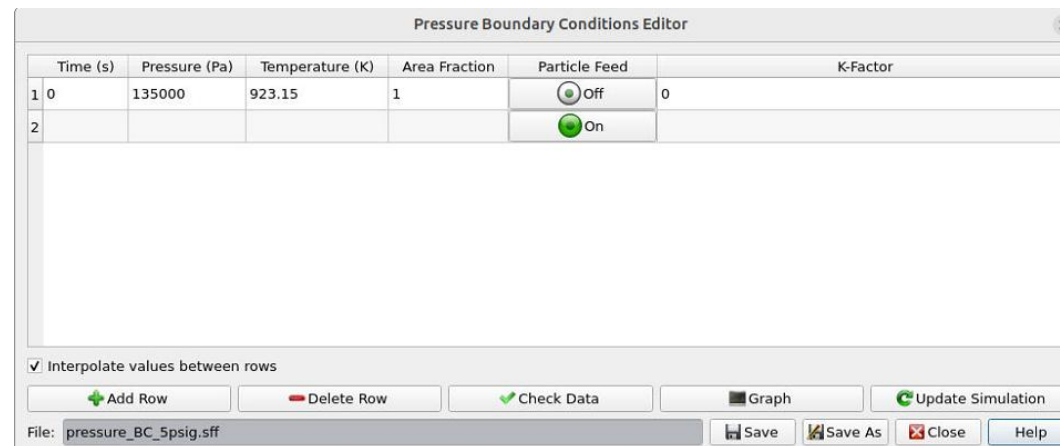
☐ Bin by particle size 100 bins

☐ Output raw particle data

☐ Output tracer data

Comment: Top of reactor boundary condition

Help Cancel OK



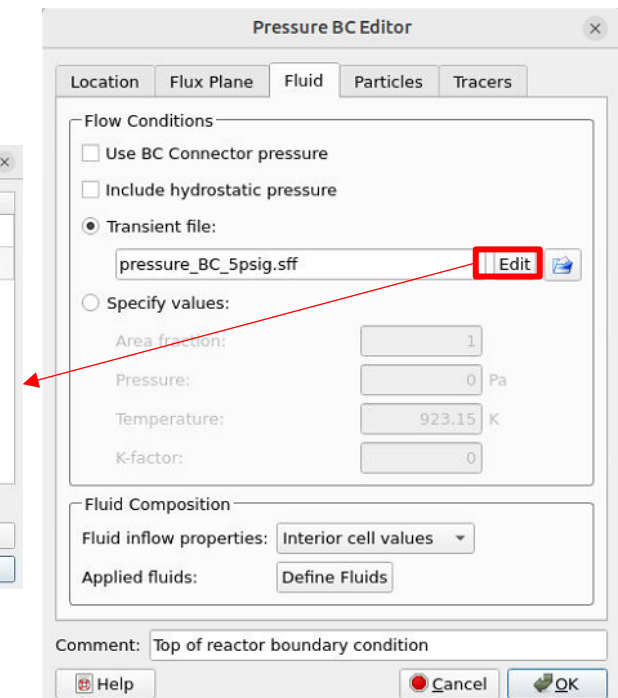
Pressure Boundary Conditions Editor

	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	

☒ Interpolate values between rows

Add Row Delete Row Check Data Graph Update Simulation

File: pressure\_BC\_5psig.sff Save Save As Close Help



Pressure BC Editor

Location: Flux Plane | Fluid | Particles | Tracers

Flow Conditions

☐ Use BC Connector pressure

☐ Include hydrostatic pressure

☒ 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

Help Cancel OK

# Flow BC

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

Gas flows in at 100 °C (373.15 K)

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)

x<sub>min</sub> min x<sub>max</sub> max

y<sub>min</sub> min y<sub>max</sub> max

z<sub>min</sub> min z<sub>max</sub> 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

User-defined Expression

☐ Select by expression Edit

Transient File

flow\_BC\_fluidizing\_gas\_inlet\_57.sff Edit

Comment: Fluidizing gas inlet containing silane and h2 mixture

Help Cancel OK

**Flow BC Editor**

Location | Flux Plane | Fluid | Particles | Tracers

Name: FLUXBC\_flow\_fluidizing\_gas

Fluid species behavior:

Mass time cumulative

☐ Bin by particle size 100 bins

☐ Output raw particle data

☐ Output tracer data

Transient File

flow\_BC\_fluidizing\_gas\_inlet\_57.sff Edit

Comment: Fluidizing gas inlet containing silane and h2 mixture

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-04	373.15	135800
3				

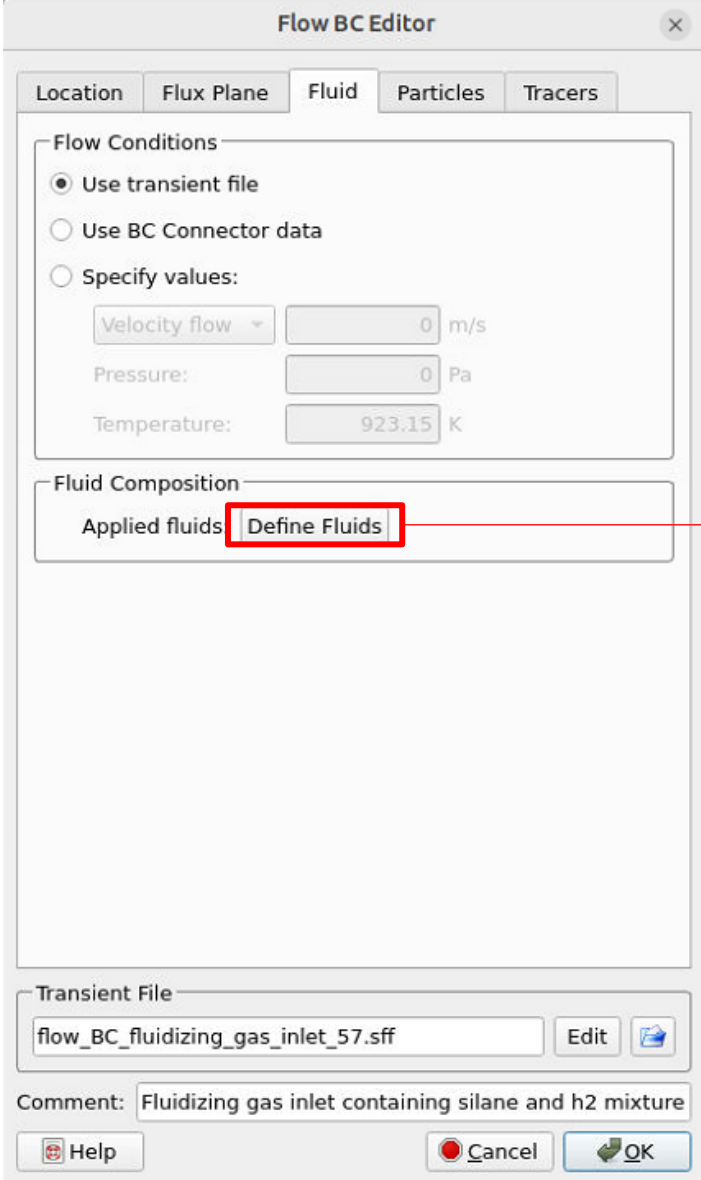
☒ Interpolate values between rows

+ Add Row - Delete Row ✓ Check Data Graph Update Simulation

File: flow\_BC\_fluidizing\_gas\_inlet\_57.sff Save Save As Close Help

# Flow BC

Use 0.57 mole fraction SiH<sub>4</sub> and 0.43 mole fraction H<sub>2</sub> under Defined Fluids.



The Flow BC Editor dialog box is shown with the 'Fluid' tab selected. It contains sections for Flow Conditions, Fluid Composition, and Transient File. A red box highlights the 'Define Fluids' button in the Fluid Composition section, with a red arrow pointing to the Mixture dialog box.

**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**

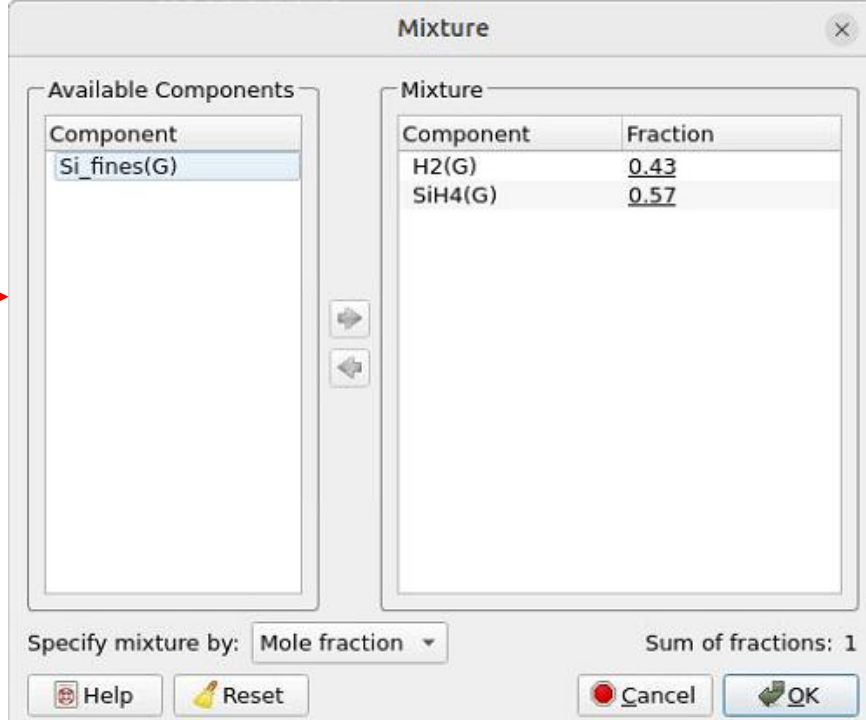
Applied fluids: **Define Fluids**

**Transient File**

flow\_BC\_fluidizing\_gas\_inlet\_57.sff [Edit] [File Icon]

Comment: Fluidizing gas inlet containing silane and h2 mixture

[Help] [Cancel] [OK]



The Mixture dialog box is shown with the 'Mixture' tab selected. It contains a table for the mixture components and a 'Specify mixture by' dropdown menu. The 'Mixture' table lists H2(G) with a fraction of 0.43 and SiH4(G) with a fraction of 0.57. The 'Specify mixture by' dropdown is set to 'Mole fraction'.

**Mixture**

Available Components

Component
Si_fines(G)

Mixture

Component	Fraction
H2(G)	0.43
SiH4(G)	0.57

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

$\theta_f$ : 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:  $c_0 T^{c_1} p^{c_2} \rho_f^{c_3} \theta_f^{c_4} e^{-E/T+E_0} \{type_s\}$

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

Values

$C_0$  = 2.793e+06

$C_1$  = 0

$C_2$  = 0

$C_3$  = 0

$C_4$  = -1

$C_5$  = 0

E = 19540

E0 = 0

Temperature unit:

Pressure unit:

Density unit:

Diameter unit:

Mass unit:

Area unit: **m<sup>2</sup>/m<sup>3</sup>**

type<sub>s</sub> = **Particle Dependence**

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

Project Materials List

Material name	Phase	Description
all		Add all particles
Si	S	

<-- Import

<-- Replace

Material Properties Library

Help 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:

SiH4 ==> Si(S) + 2 H2

Check Add Material

Expected Power Law rate equation format:  $c_0 (k + k - \dots) [material1]^{\text{power}} [material2]^{\text{power}} + c_1 \dots$   
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:  $(c_0 k [ ] + c_1 k [ ] + \dots) / (1 + c_2 k [ ] + c_3 k [ ] + \dots)^{\text{power}}$   
Example of groups of rates:  $(c_0 k_0 [O_2] - c_1 (0.5k_1 - k_2))^{1.5} (c_1 k_3) [CO]^{0.5} [O_2]^{-1}$

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

R00 = (k0[SiH4])

Check Add Volume-Average Coefficient Add Material Coefficients Manager

Comment  
Direct deposition through heterogeneous reaction

Help Cancel OK

Chemistry Reactions Manager

ID	Reaction Type	Rate	Equation	Comment
00	VA: Stoichiometric	Equation: $SiH_4 ==> Si(S) + 2 H_2$ R00 = $(k_0[SiH_4])$		Direct deposition through heterogeneous reaction
01	VA: Stoichiometric	Equation: $SiH_4 ==> Si_{fines} + 2 H_2$ R01 = $(k_1[SiH_4])$		Homogeneous decomposition of silane
02	VA: Stoichiometric	Equation: $Si_{fines} ==> Si(S)$ 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.

Visualization Data Output

Output file format:  
☒ Tecplot (\*.plt files) ☐ GMV (Gmv.\* files)

Output file interval:  
☒ Constant:  s End time: 150s Number of output files: 151  
☐ Time-varying:  Edit

Cell Data

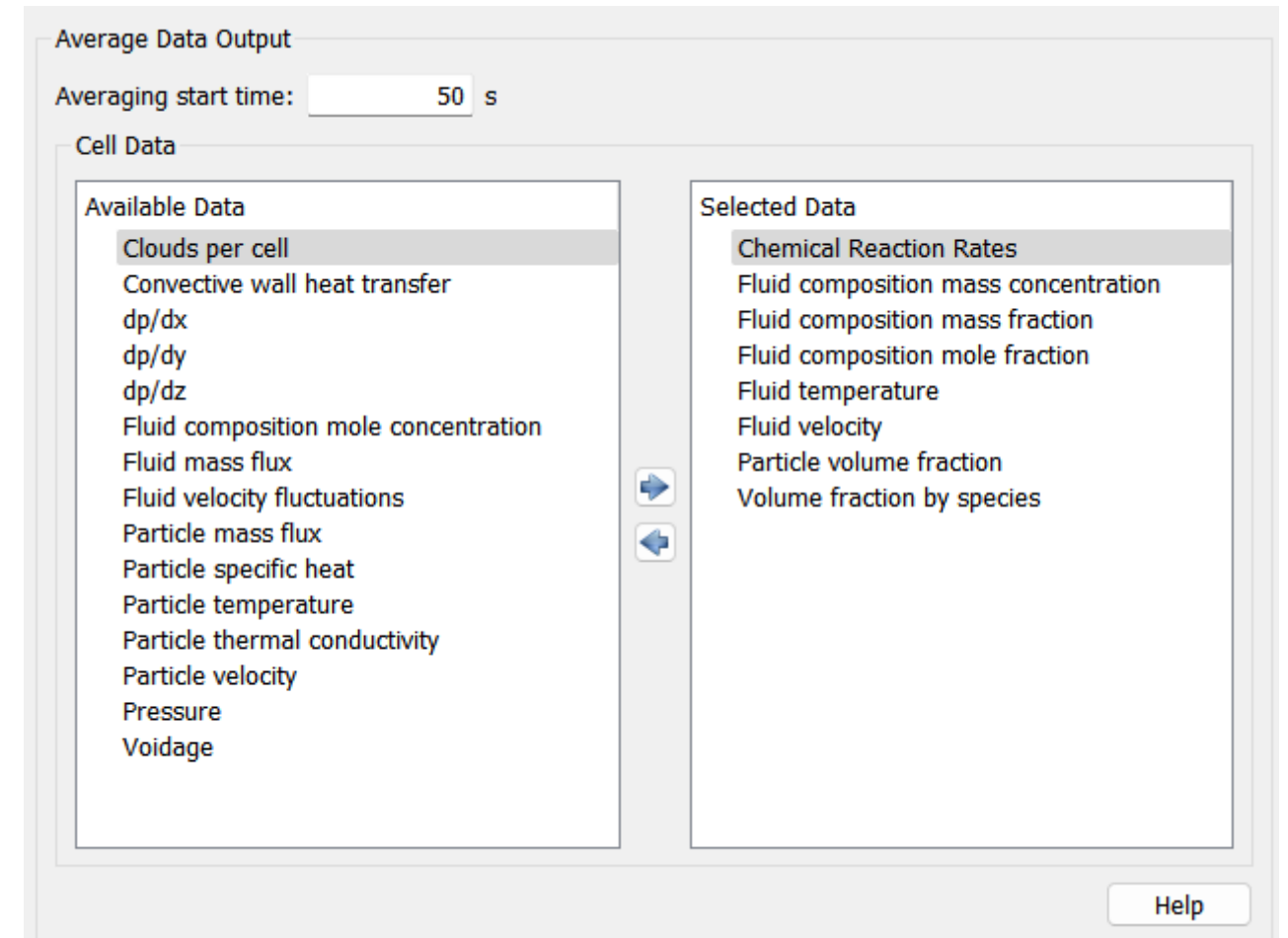
Available Data		Selected Data
Cell ID		Bulk density
Clouds per cell		Cell indices
Convective wall heat transfer		Cell volume
dp/dx		CFL
dp/dy		Chemical Reaction Rates
Dynamic pressure		dp/dz
Fluid composition mass concentration		Fluid composition mass fraction
Fluid composition mole concentration		Fluid composition mole fraction
Fluid mass flux		Fluid density
P1 incident radiation flux		Fluid temperature
P1 radiation flux		Fluid velocity
P1 radiation flux from walls		Particle volume fraction
P1 radiation to fluids		Pressure
P1 radiation to particles		
Particle mass flux		
Particle temperature		
Particle velocity		

Particle Data

Available Data		Selected Data
Cell ID		Chemical Reaction Rates
Drag		Cloud ID
Liquid fraction total		Cloud mass
Liquid mass total		Particle density
P1 radiation flux		Particle mass
Particle material		Particle size
Particle velocity		Particle speed
Particles per cloud		Particle temperature
Residence time		Particle volume fraction
Species		

# Average Data Output

Select the following outputs under the  
Average Data window

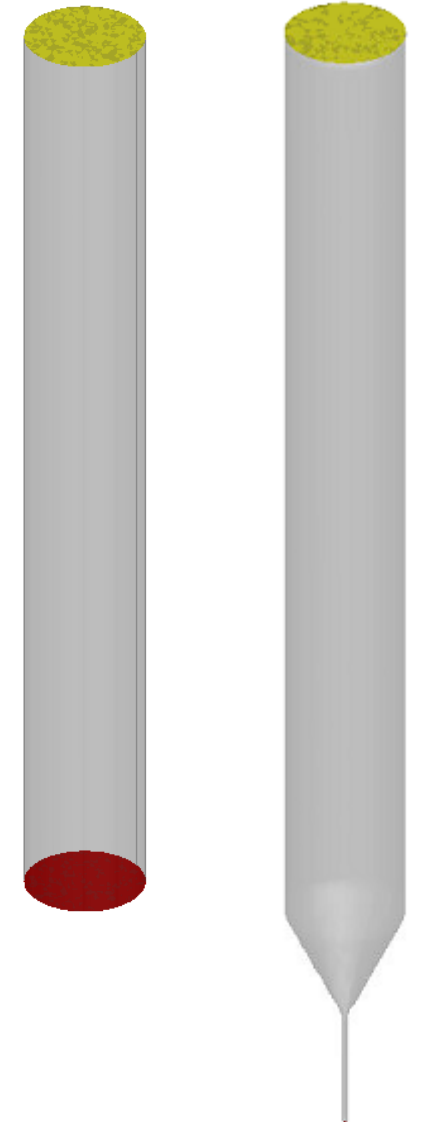
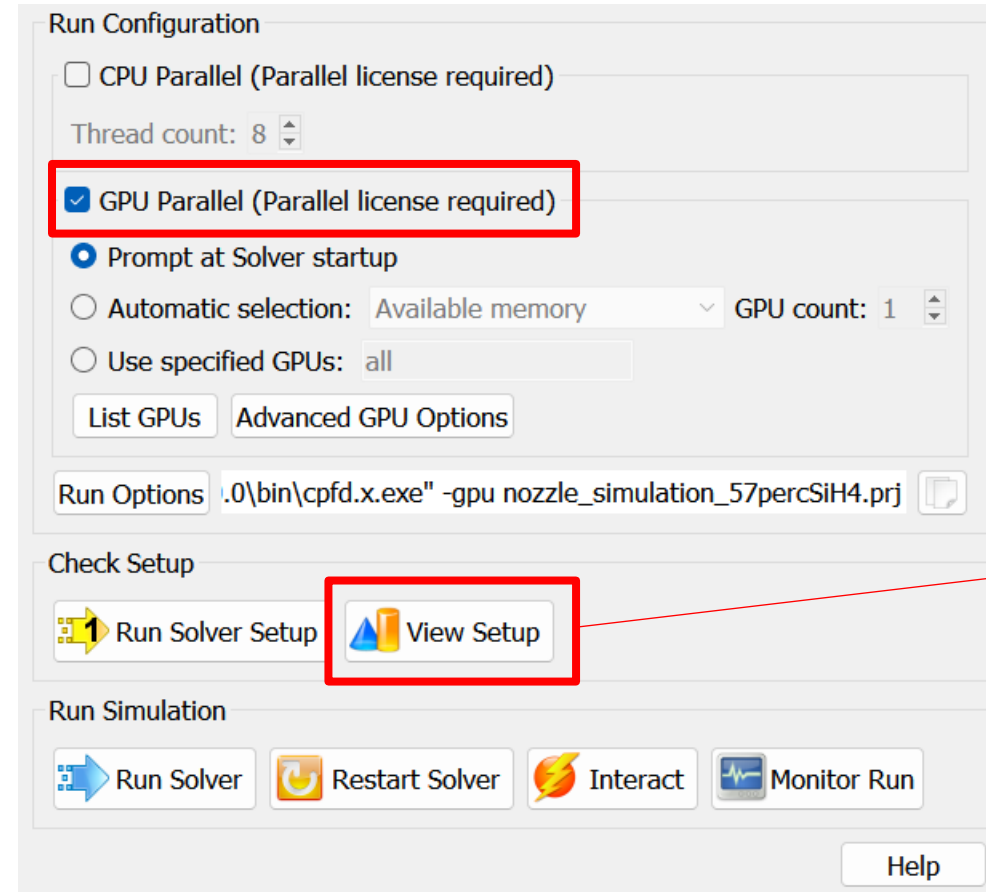


# Run

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



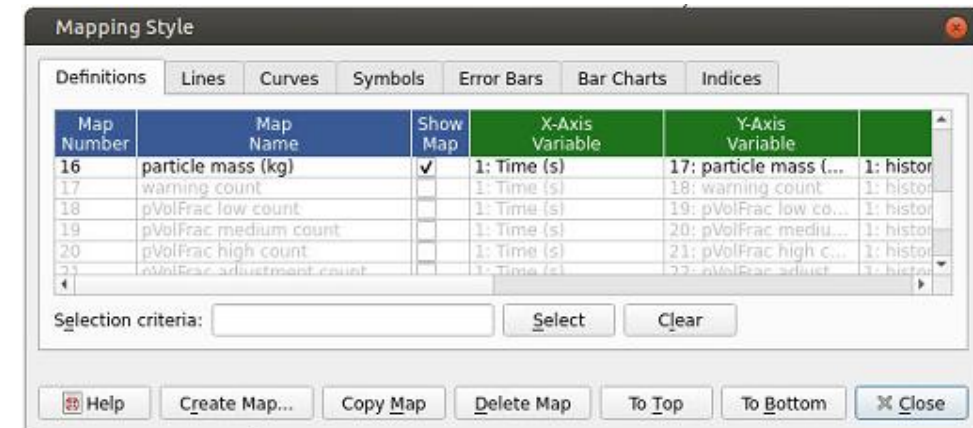
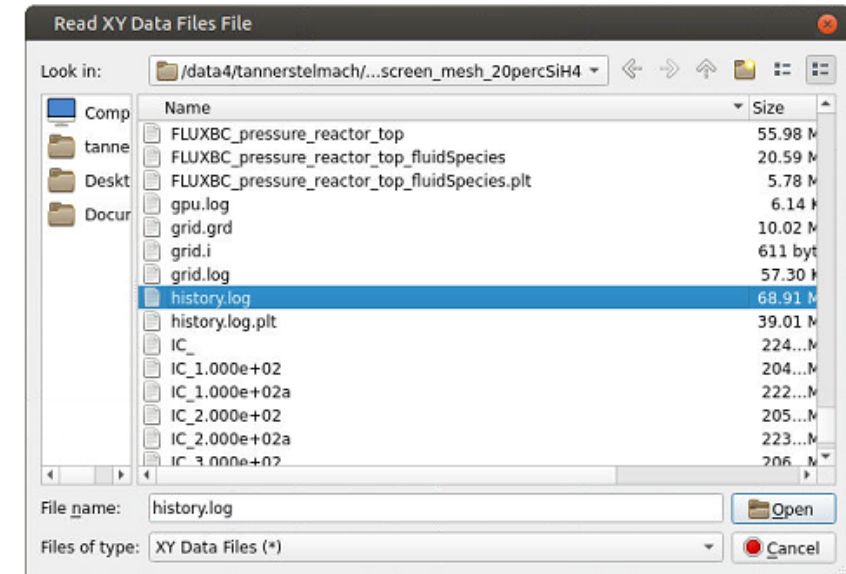


# Post-Processing: Silicon Deposition Rate

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



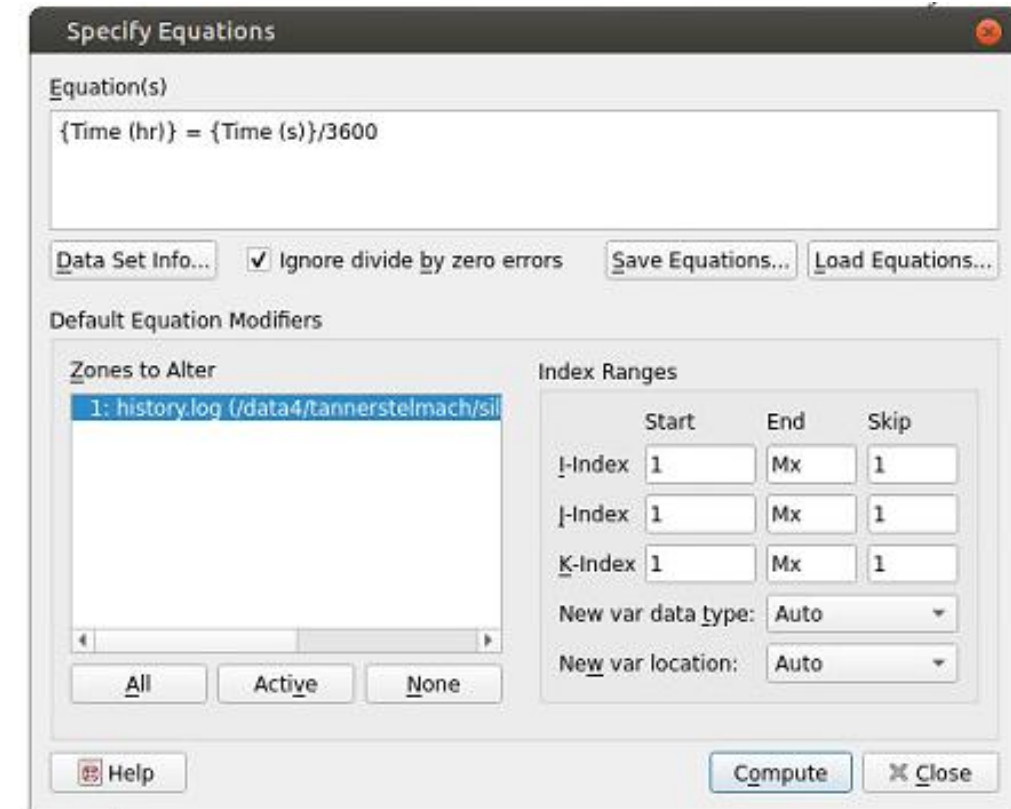


# Post-Processing: Silicon Deposition Rate

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*



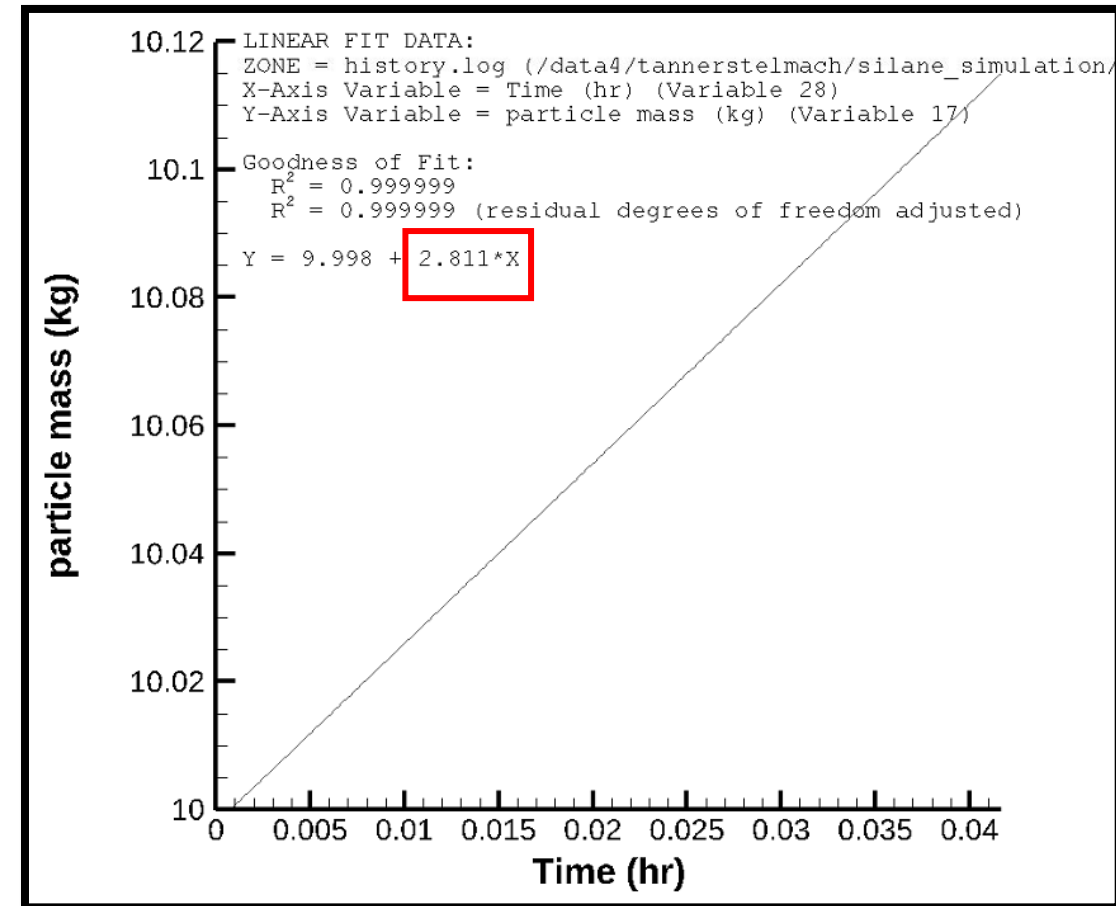
# Post-Processing: Silicon Deposition Rate

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



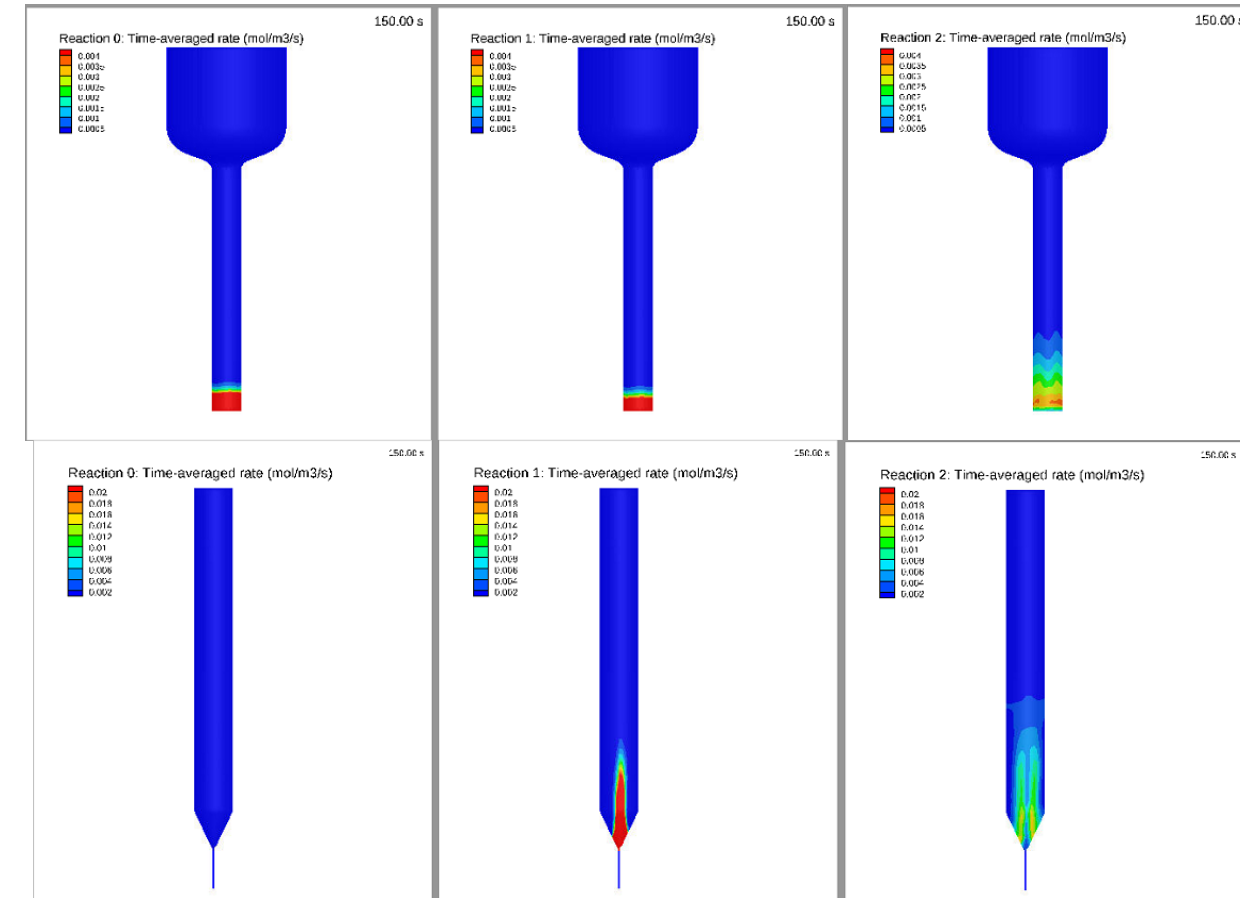
# Post-Processing: Reaction Rate Output

## 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/>

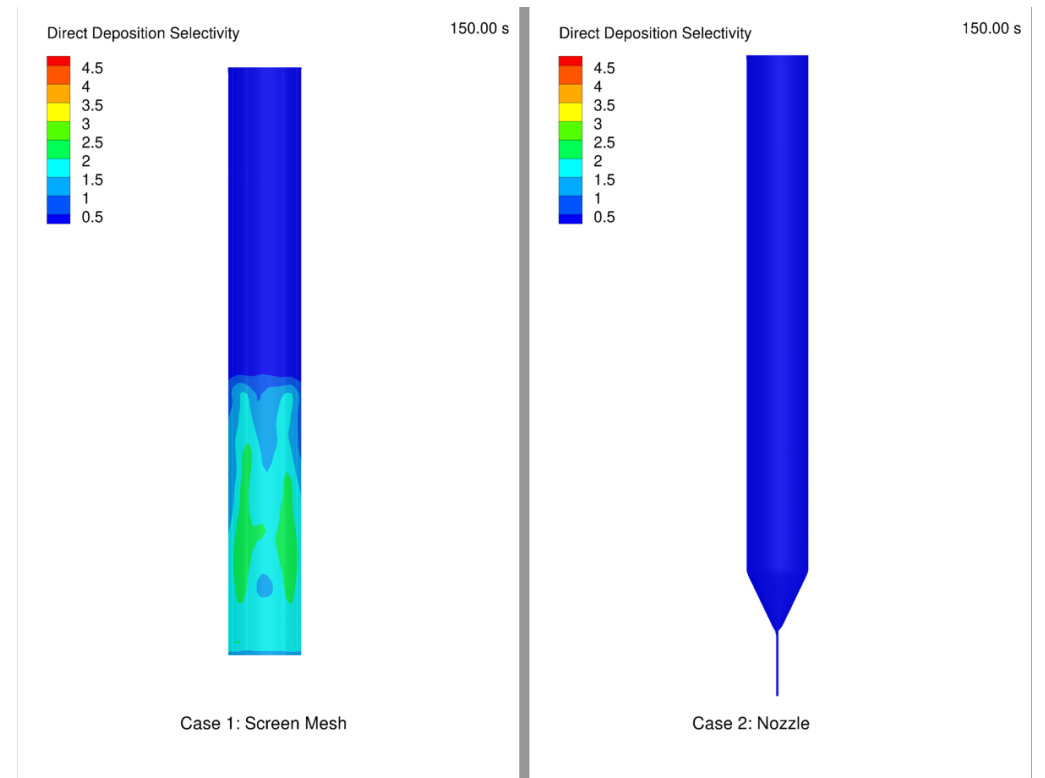


# Post-Processing: Direct Deposition Reaction Selectivity

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*

**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

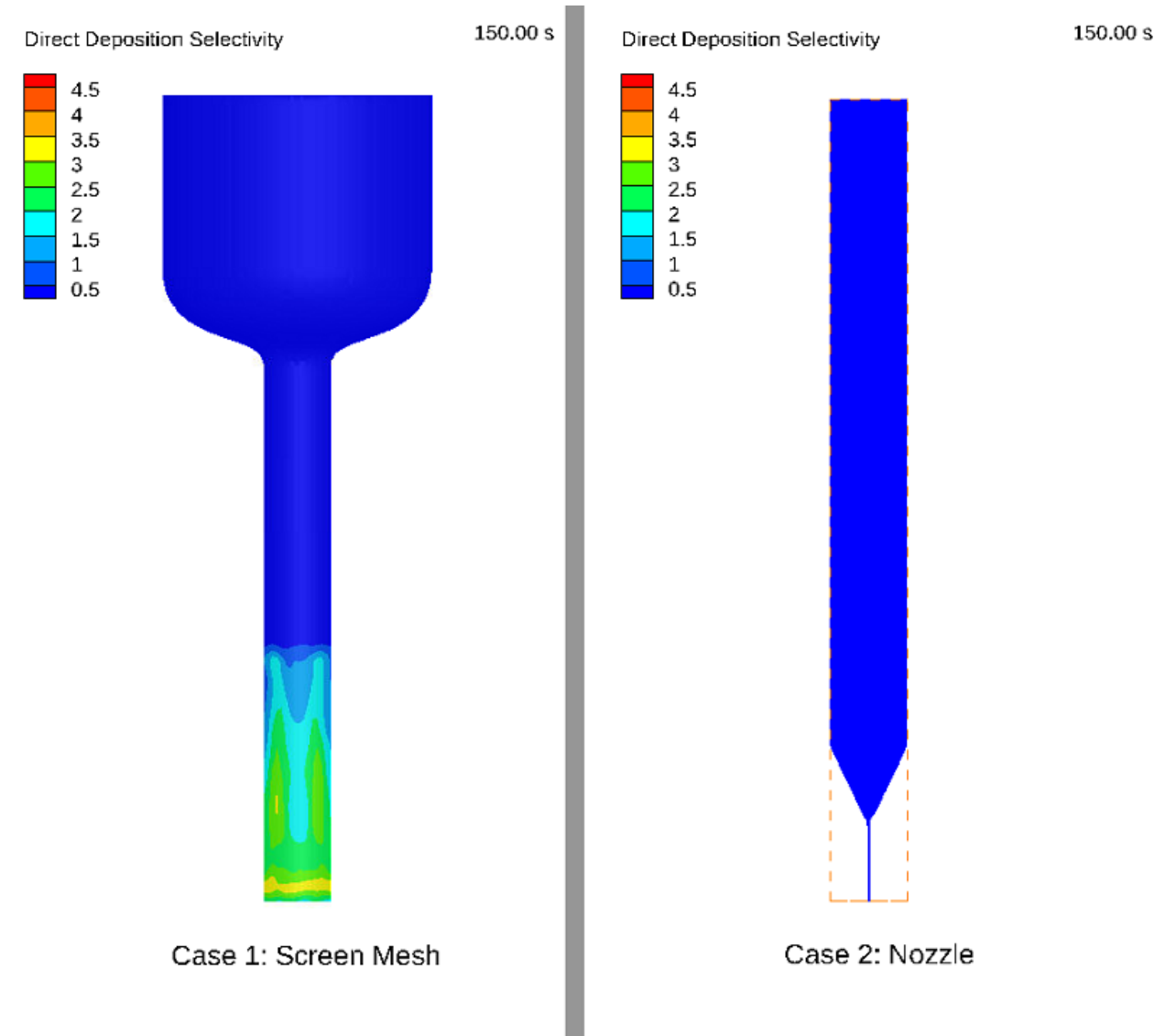
Help Compute Close

# Create a slice and select the appropriate data

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

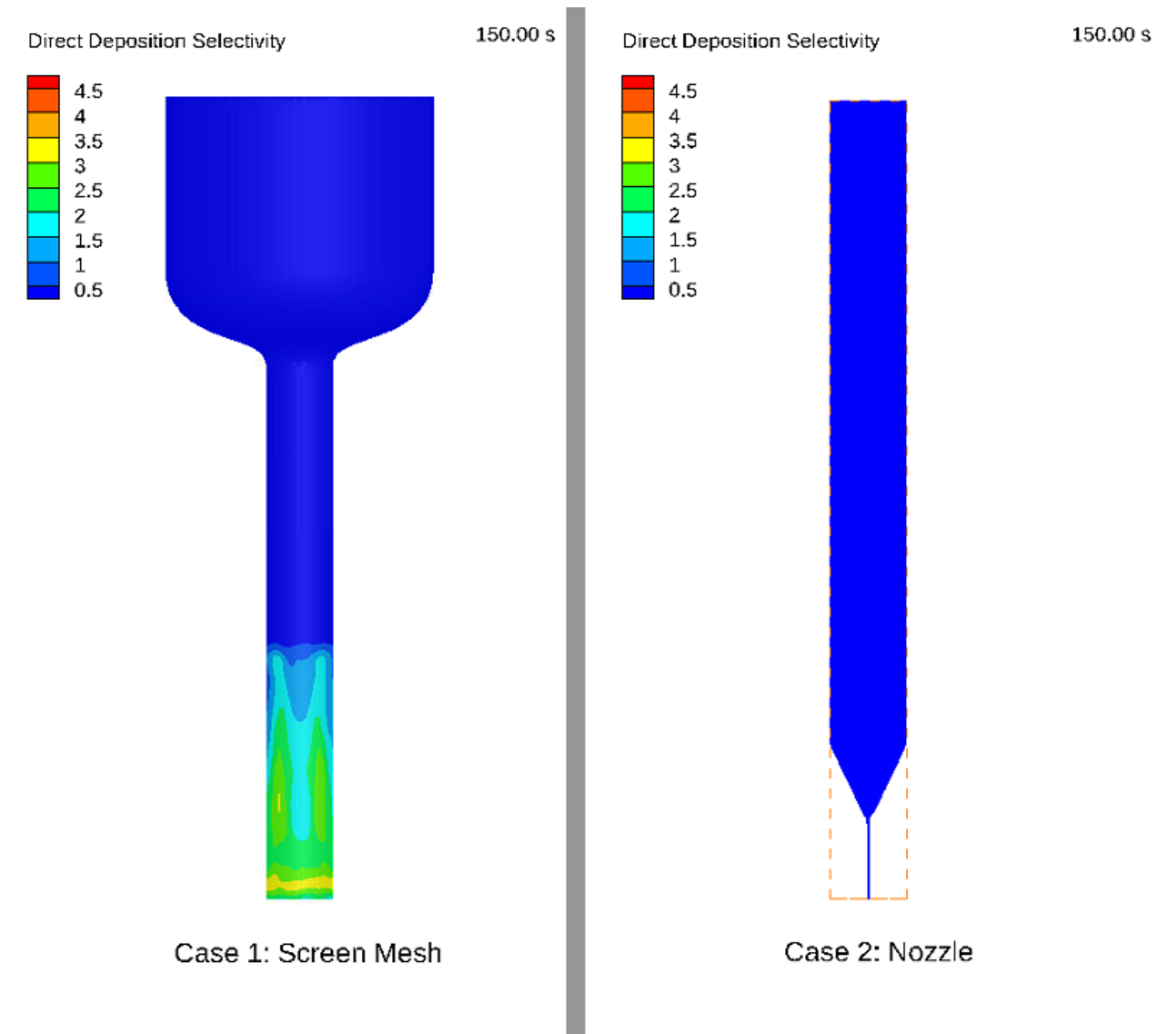
Adjust the color bar to the desired view. Here we use *Modified Rainbow (less green)*

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.

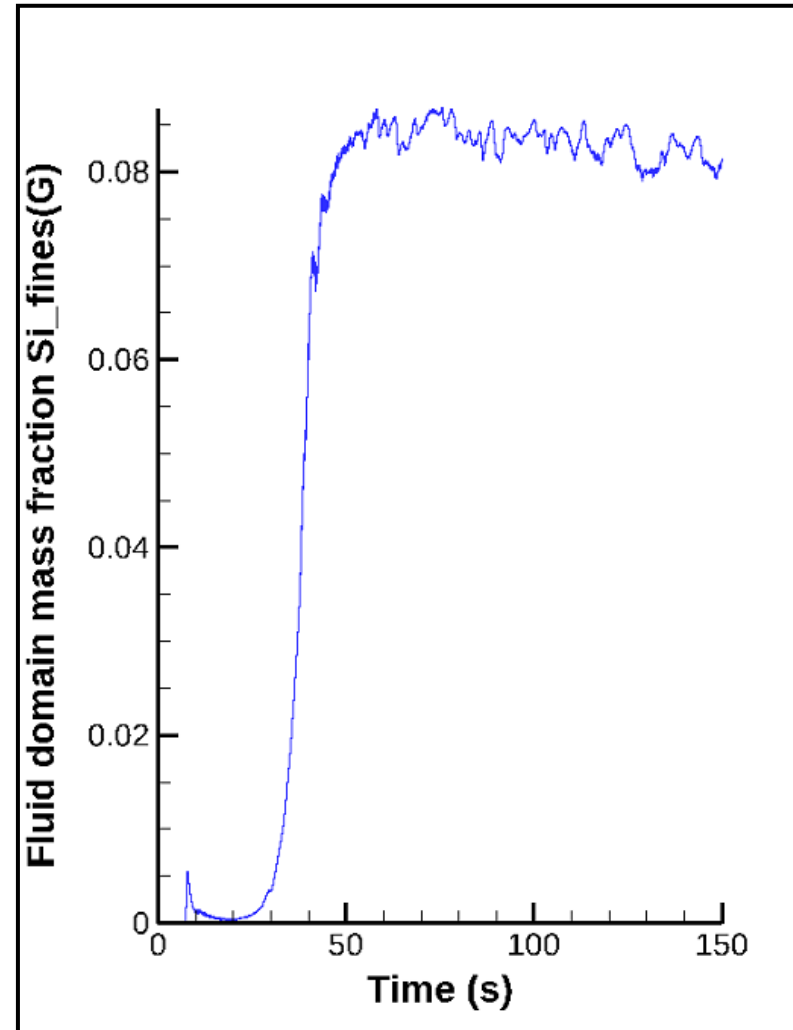
First, select *Launch Tecplot*, then *File / Load Barracuda Data/ Load Data File/ FLUXBC\_pressure\_reactor\_top\_fluidSpecies*. This will open the Flux file at the reactor top



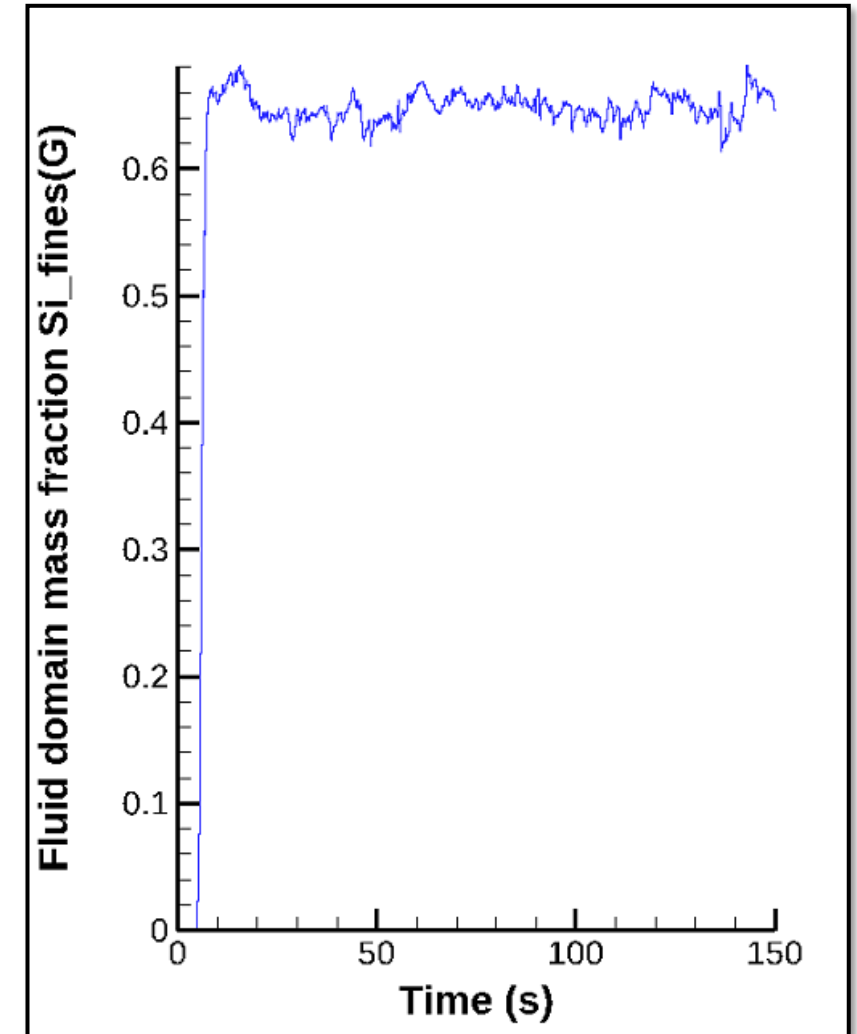
# Post-Processing: Silicon Fines Exit Mass Fraction

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  $\text{SiH}_4$ ). 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 $\text{SiH}_4$ (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

SaveSave AsCloseHelp

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

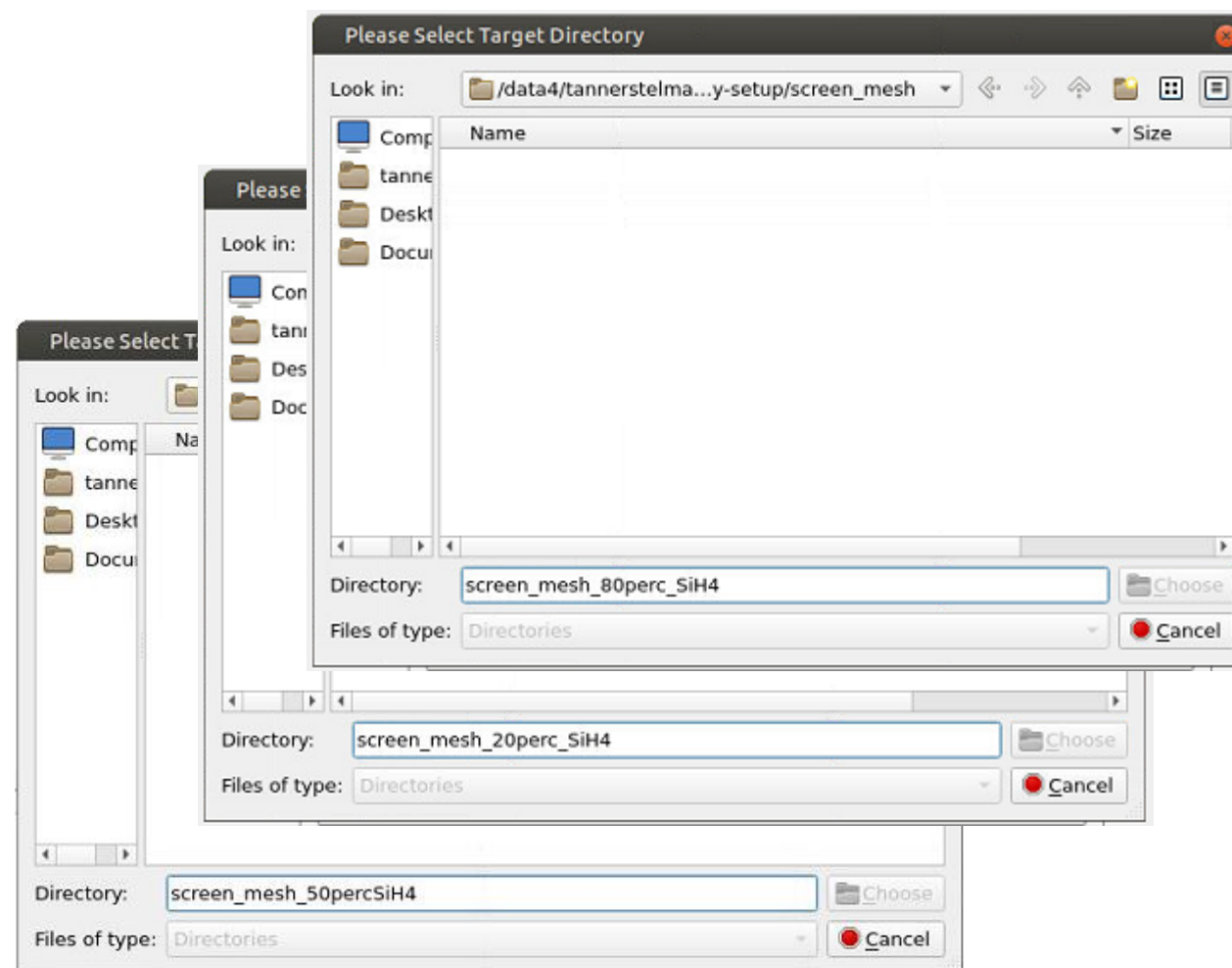
HelpResetCancelOK

# Test other feed fractions of SiH<sub>4</sub> 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% SiH<sub>4</sub>**

Notes: In the *pre-setup* folder, the additional cases can be run by substituting the sff files contained (under *sff\_files directory*) in order to run with different silane feed fractions.



## 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

