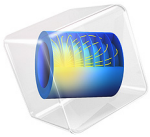

Surface Chemistry Tutorial Using the Plasma Module

Introduction

Surface chemistry is often the most important and most overlooked aspect of reacting flow modeling. Surface rate expressions can be hard to find or not even exist at all. Often it is preferable to use sticking coefficients to describe surface reactions because they can be estimated intuitively.

Model Definition

The tutorial model simulates outgassing from a wafer during a chemical vapor deposition (CVD) process. Careful attention is paid to the overall mass balance in the system and the difference between the mass averaged velocity and diffusion velocity is explored.

The same physical problem is investigated first with a global (volume-averaged) model and after with a space dependent model. An initial study of a problem with a global model is a good approach when there is limited knowledge about the system. One reason is that the global model has reduced computational times, allowing for fast sweeps over parametric spaces. The fast computational time of global models is also a great advantage to investigate models with complex chemistries.

In some cases a volume–averaged model might even be good enough to extract the desired information from the model. If, however, space dependent information is necessary, a space dependent model can be implemented in a subsequent study.

The geometry and operating principle for the model is shown in Figure 1. Initially the closed container is full of 99.9% silicon hydride and 0.1% hydrogen (measured by molar content).

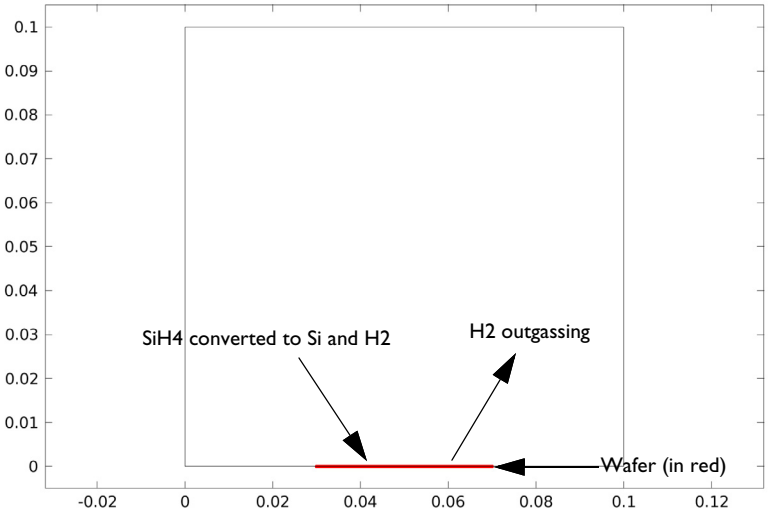

Figure 1: Geometry and basic operating principle for the surface chemistry tutorial model.

A surface reaction begins to occur on the wafer which consumes the silicon hydride, releases hydrogen into the domain, alters the composition of the absorbed species on the wafer surface and deposits bulk silicon. The following reactions are considered on the surface of the wafer:

TABLE 1: SURFACE REACTIONS CONSIDERED.

REACTION	STICKING COEFFICIENT OR RATE CONSTANT
SiH4+2Si(s)=>Si(b)+2SiH(s)+H2	2E-4
SiH(s)=>Si(s)+0.5H2	3 1/s

The (s) here denotes "surface species" which means that the species only exists on the surfaces where the reaction is occurring. To indicate that a species is bulk, append (b) to the end of the species. Since bulk species cannot participate in surface reactions, they must only be products and not reactants in a surface reaction. The net result of these two competing reactions is `SiH4=>Si(b)+2H2`, which means it is expected that the silane is replaced by hydrogen inside the reactor, and layers of silicon deposited on the wafer surface.

MODEL EQUATIONS — SURFACE REACTIONS AND SURFACE SPECIES

The surface reaction rate for reaction i is given by:

$$q_i = k_{f,i} \prod_{k=1}^{K} c_k^{\nu_{ki}^f} - k_{r,i} \prod_{k=1}^{K} c_k^{\nu_{ki}^r}$$

where c_k is the molar concentration of species k. The rate constant k_f can be given by

$$k_{\mathrm{f},i} = \left(\frac{\gamma_i}{1-\gamma_i/2}\right) \frac{\prod \sigma_j^{\nu_{ji}}}{(\Gamma_{\mathrm{tot}})^m} \left(\frac{1}{4}\right) \sqrt{\frac{8RT}{\pi M_k}}$$

where Γ_{tot} is the total surface site concentration (SI unit: mol/m^2), m is the reaction order minus 1, T is the surface temperature, R is the gas constant, M_k is the molecular weight, and γ_i is the sticking coefficient. When defining a surface reaction that contains no gas-phase reactants consider specifying the reaction using a rate coefficient. Otherwise, if using the equation above the mean gas-phase molecular weight is used.

For the surface species the following equations are solved:

$$\frac{dZ_k}{dt} = \frac{R_{\mathrm{surf},k}}{\Gamma_{\mathrm{tot}}}$$

where Z_k is the site fraction (dimensionless), $R_{\mathrm{surf},k}$ is the surface rate expression (SI unit: mol/m^2). The quantity Z_k is the surface equivalent of the mole fraction on the volumetric level. That is, the sum of the site fractions must always equal one:

$$\sum Z_k = 1\,.$$

Empty sites are not accounted for in reaction rate coefficients, so all species which can occupy a surface must be included in the model. The surface site concentration is given by:

$$c_k = \frac{Z_k \Gamma_{\mathrm{tot}}}{\sigma_k}\,.$$

For each of the bulk surface species, the following equation is solved for the deposition height:

$$\frac{dh_k}{dt} = -\frac{R_{\mathrm{surf},k} M_k}{\rho_k}$$

where h_k is the total growth height (SI unit: m), M_k is the molecular weight (SI unit: kg/mol), and ρ is the density of the bulk species (SI unit: kg/m^3).

DOMAIN EQUATIONS

Inside the domain, the Navier-Stokes equations are solved for the fluid velocity. The mass fraction of hydrogen is computed by solving:

$$\rho\frac{\partial}{\partial t}(w) + \rho(\mathbf{u}\cdot\nabla)w = \nabla\cdot\mathbf{j}$$

where w is the mass fraction of hydrogen. For detailed information on the transport of the nonelectron species see *Theory for the Heavy Species Transport Interface* in the *Plasma Module User's Guide*. The mass fraction of silane is not directly computed. Its value comes from the fact that the sum of the mass fractions must equal one. The gas temperature is computed by solving the energy equation.

BOUNDARY CONDITIONS

Fluid Flow

The following boundary conditions are used. The mass averaged velocity is constrained using:

$$\mathbf{u} = -\frac{M_f}{\rho}\mathbf{n}$$

where M_f is the inward (or outward in this example) mass flux which is defined, from the surface chemistry as:

$$M_f = \sum_{k=1}^{K_g} M_k \dot{s}_k$$

where s_k is the surface rate expression for each species which comes from summing the surface reaction rates multiplied by their stoichiometric coefficients over all surface reactions:

$$\dot{s}_k = \sum_{i=1}^{I} \nu_{ki} q_i$$

Hydrogen Mass Fraction

The flux of hydrogen at the surface of the wafer comes from the surface reactions:

$$\mathbf{n} \cdot \mathbf{j} = M_k s_k$$

Energy Equation

For the energy equation, the following boundary condition is used:

$$\mathbf{n} \cdot \kappa \nabla T = \sum_{i=1}^{I} q_i h_i$$

where hi is the molar enthalpy change due to reaction i.

GLOBAL MODEL EQUATIONS

The global model used in this work considers that the spatial information of the different quantities in the plasma reactor can be treated as uniform. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is reduced. For detailed information on the global model see *Theory for the Heavy Species Transport Interface* in the *Plasma Module User's Guide*. For heavy species, the following equation is solved for the mass fraction:

$$V\rho\frac{d}{dt}(w_k) = VR_k + \sum_l h_l A_l R_{surf,k,l} M_k - w_k \sum_l h_l A_l M_{f,l}$$

where ρ is the mass density (SI unit: kg/m^3), w_k is the mass fraction, and R_k is the rate expression (SI unit: kg/(m^3.s)). The fourth term on the right hand side accounts for surface losses and creation, where A_l is the surface area, h_l is a dimensionless correction, V is the reactor volume, M_k is the species molar mass (SI unit: kg/mol) and $R_{surf,k,l}$ is the surface rate expression (SI unit: mol/(m^2.s)) at a surface l. The last term on the right-hand side is introduced because the species mass balance equations are written in the nonconservative form and it used the mass-continuity equation to replace for the mass density time derivative. In the last term, $M_{f,l}$ is the inward mass flux of surface l (SI unit: kg/(m^2·s)). The sum in the last two terms is over all surfaces where there are surface reactions.

To take into account possible variations of the system total mass or pressure, the mass-continuity equation is also solved:

$$V\frac{d\rho}{dt} = \sum_l h_l A_l M_{f,l}\,.$$

The gas temperature is set to a constant value. The model for the surface chemistry is exactly the same.

Results and Discussion

In this section, both space-dependent and global model results are presented and discussed. For this particular physical system, the results from the global model and the space dependent model are in a very good agreement.

The y-component of the mass-averaged velocity is plotted in Figure 2. The mass-averaged velocity is negative at the surface of the wafer. This means that overall, mass is leaving the system. This is to be expected since silane is being consumed, which has a molecular weight of 0.032 kg/mol and replacing it with hydrogen, which has a lower molecular weight of 0.002 kg/mol.

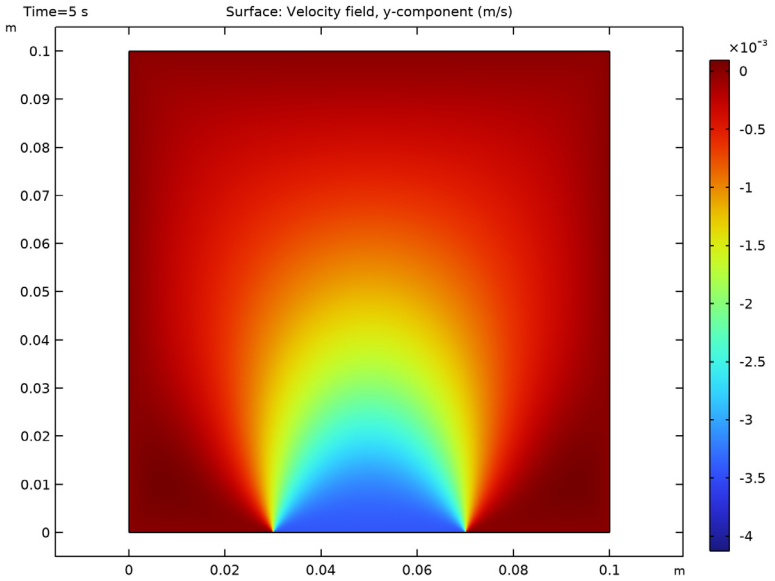

Figure 2: Plot of the mass averaged velocity field after 5 seconds.

The surface reactions begin to consume the silane, which results in concentration gradients within the reactor. The outward mass flux at the wafer surface leads to a mass-averaged velocity everywhere inside the reactor. The combination of concentration gradients and convection due to the mass-averaged velocity tends to draw silane toward the wafer. The first surface reaction is exothermic while the second surface reaction is endothermic. The amount of heat released by the exothermic reaction dominates, so the temperature begins to increase. The temperature is plotted in Figure 3 and is highest on the wafer surface.

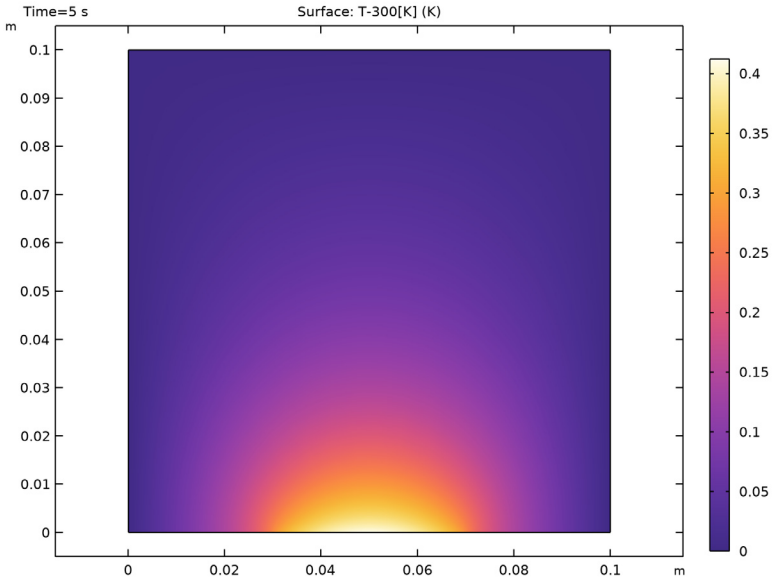

Figure 3: Plot of the change in gas temperature after 5 seconds. The higher temperature is observed at the wafer surface due to the heat released in the surface reactions.

From the net reaction `SiH4=>Si(b)+2H2` there should be a molar inflow of hydrogen at twice the rate that silane is leaving. Although this condition is not applied explicitly, it is implicit from the equations solved in the Heavy Species transport interface. Despite the fact that there is a negative mass-averaged velocity, there is a positive diffusion velocity for the hydrogen at the wafer surface. The y-component of the diffusion velocity for hydrogen is plotted in Figure 4.

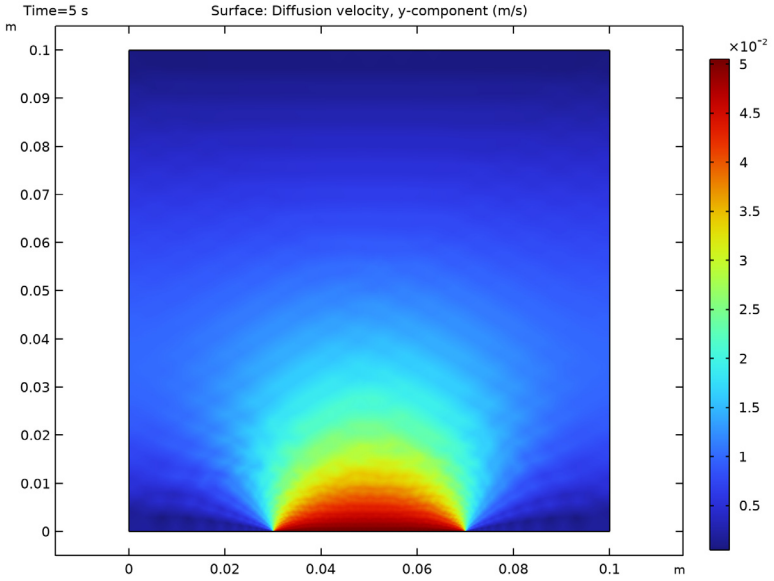

Figure 4: Plot of the y-component of the diffusion velocity for hydrogen after 5 seconds. Even though the mass-averaged velocity is negative, the diffusion velocity is positive, indicating an inflow of hydrogen and a net outflow of total mass.

Figure 5 plots the integrated pressure in the reactor divided by the initial average pressure in the reactor. Once the problem reaches steady state, the average pressure in the reactor has increased by a factor of 2. This is expected since every mole of silane is being replaced by two moles of hydrogen. The silane in the reactor is completely consumed after around 200 seconds.

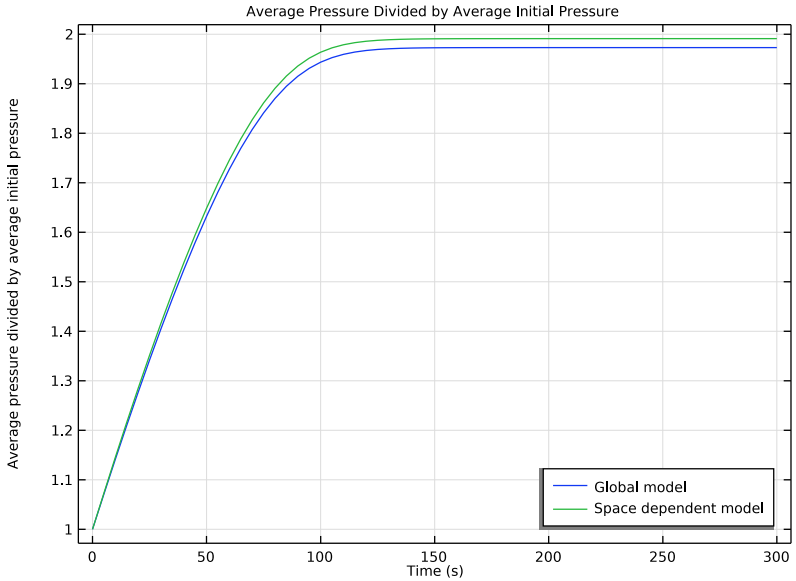

Figure 5: Plot of the ratio of the average pressure by the average initial pressure computed with the global model (blue) and the space dependent model (green).

In Figure 6, the total mass initially present in the reactor divided by the total mass in the reactor is plotted. The total mass in the reactor drops by a factor of 8, which is expected since the silane with molecular mass 0.032 kg/mol is replaced with two moles of hydrogen, which has a molecular weight of 2·0.002=0.004 kg/mol.

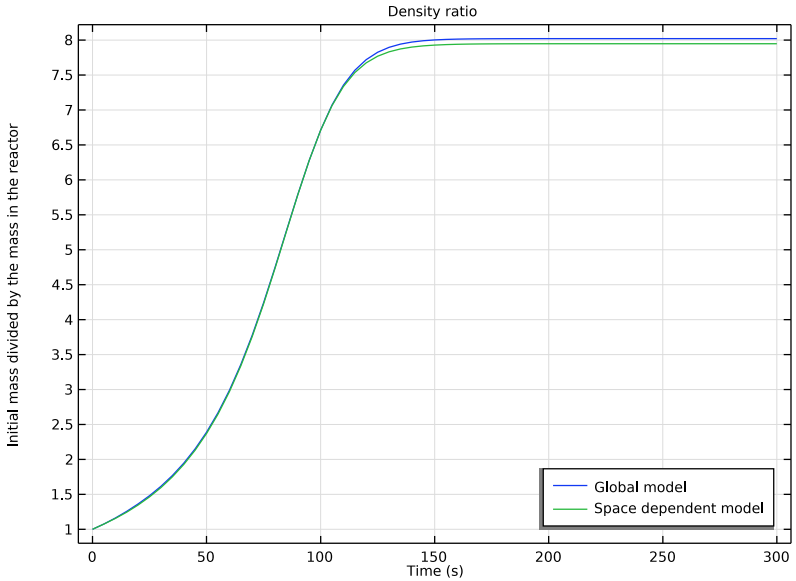

Figure 6: Plot of the ratio of the total mass by the total mass computed with the global model (blue) and the space dependent model (green).

Another way of verifying the correctness of the model is to compare the mass lost inside the reactor to the mass accumulated on the wafer surface. The two quantities should be equal. The total gain in mass from surface and bulk species is compared to the total loss in mass from the reactor in Figure 7. The two curves agree very well, indicating that the total mass in the entire system is conserved.

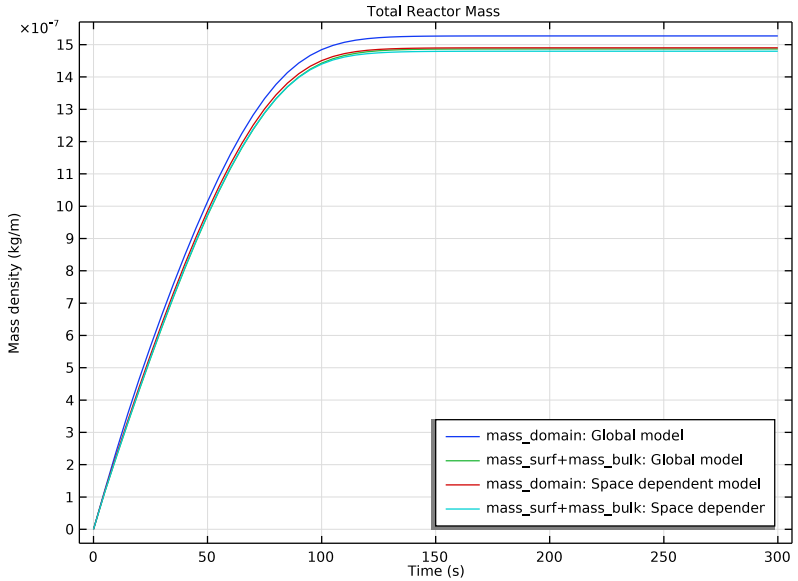

Figure 7: Plot of the total mass lost in the domain (blue: global model, and red: space dependent model) and the total mass gained due to Silicon deposition on the wafer surface (green: global model and cyan: space dependent model).

The ultimate goal of most CVD models is to determine the total growth height and growth rate on the surface of the wafer. The total growth height is plotted in Figure 8 and saturates at about 159 angstroms. The total growth rate saturates because all the silane in the reactor is consumed after around 200 seconds. The accumulated growth height is also very uniform across the surface of the wafer. The global model and space dependent model results for the total growth height agrees very well (not shown).

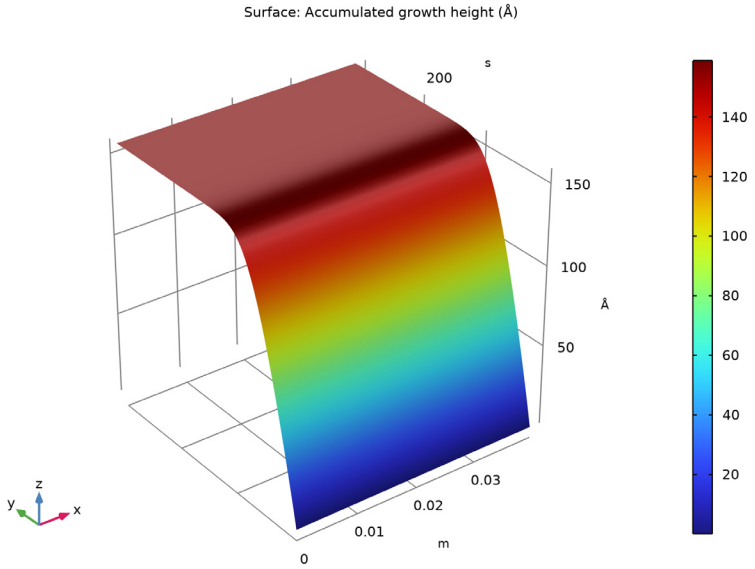

Figure 8: Plot of the growth height (surface and z-axis) versus the wafer arc length (x-axis) and time (y-axis). The final height of deposited silicon is 158 Å.

Reference

1. R.J. Kee, M.E. Coltrin, and P. Glarborg, *Chemically Reacting Flow Theory and Practice*, John Wiley & Sons, 2003.

Application Library path: `Plasma_Module/Chemical_Vapor_Deposition/surface_chemistry_tutorial`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Plasma>Species Transport>Heavy Species Transport (hs)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Square 1 (sq1)

1 In the **Geometry** toolbar, click **Square**.

2 In the **Settings** window for **Square**, locate the **Size** section.

3 In the **Side length** text field, type `0.1`.

Polygon 1 (pol1)

1 In the **Geometry** toolbar, click **Polygon**.

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 In the table, enter the following settings:

x (m)	y (m)
0.03	0
0.07	0

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `surface_chemistry_tutorial_variables.txt`.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 Select Domain 1 only.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

HEAVY SPECIES TRANSPORT (HS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heavy Species Transport (hs)**.

2 In the **Settings** window for **Heavy Species Transport**, locate the **Diffusion Model** section.

3 From the **Diffusion model** list, choose **Global**.

Surface Reaction 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Surface Reaction**.

2 In the **Settings** window for **Surface Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `SiH4+2Si(s)=>Si(b)+2SiH(s)+H2`.

4 Select Boundary 4 only.

5 Locate the **Reaction Parameters** section. In the γ_f text field, type `2e-4`.

Surface Reaction 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Surface Reaction**.

2 In the **Settings** window for **Surface Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `SiH(s)=>Si(s)+0.5H2`.

4 Select Boundary 4 only.

5 From the **Specify reaction using** list, choose **Rate coefficient**.

6 Locate the **Reaction Parameters** section. In the k_s^f text field, type `3`.

Species: SiH4

1 In the **Model Builder** window, click **Species: SiH4**.

2 In the **Settings** window for **Species**, locate the **Species Formula** section.

3 Select the **From mass constraint** check box.

4 Locate the **General Parameters** section. From the **Preset species data** list, choose **SiH4**.

Species: H2

1 In the **Model Builder** window, click **Species: H2**.

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **H2**.

4 In the x_0 text field, type `1E-3`.

Species: Si(s)

1 In the **Model Builder** window, click **Species: Si(s)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Si**.

4 Locate the **Surface Species Parameters** section. In the $Z_{k,0}$ text field, type `0.995`.

Species: Si(b)

1 In the **Model Builder** window, click **Species: Si(b)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **Si**.

Species: SiH(s)

1 In the **Model Builder** window, click **Species: SiH(s)**.

2 In the **Settings** window for **Surface Species**, locate the **General Parameters** section.

3 From the **Preset species data** list, choose **SiH**.

4 Locate the **Surface Species Parameters** section. In the $Z_{k,0}$ text field, type `0.005`.

Heavy Species Model 1

1 In the **Model Builder** window, click **Heavy Species Model 1**.

2 In the **Settings** window for **Heavy Species Model**, locate the **Model Inputs** section.

3 In the p_0 text field, type `13.3`.

GLOBAL MODEL

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Global model` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

4 Clear the **Generate convergence plots** check box.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Global model** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,5,300)`.

4 In the **Home** toolbar, click = **Compute**.

RESULTS

Average Pressure Divided by Average Initial Pressure

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Average Pressure Divided by Average Initial Pressure` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global model

1 Right-click **Average Pressure Divided by Average Initial Pressure** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`hs.pA/at(0,hs.pA)`	1	

5 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Global model`

7 In the **Average Pressure Divided by Average Initial Pressure** toolbar, click **Plot**.

Density ratio

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Density ratio` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global model

1 Right-click **Density ratio** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`at(0,hs.rho)/hs.rho`	`1`	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Global model`

7 In the **Density ratio** toolbar, click **Plot**.

Total Reactor Mass

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Total Reactor Mass` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global model

1 Right-click **Total Reactor Mass** and choose **Global**.

2 In the **Settings** window for **Global**, type `Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Global model/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`mass_domain`	`kg/m`	`Mass change in the domain`
`mass_surf+mass_bulk`	`kg/m`	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`mass_domain: Global model`
`mass_surf+mass_bulk: Global model`

7 In the **Total Reactor Mass** toolbar, click **Plot**.

Edge 2D 1

1 In the **Model Builder** window, expand the **Results>Datasets** node.

2 Right-click **Results>Datasets** and choose **Edge 2D**.

3 Select Boundary 4 only.

Parametric Extrusion 1D 1

In the **Results** toolbar, click  **More Datasets** and choose **Parametric Extrusion 1D**.

Parametric Extrusion 1D 1 - Global model

1 In the **Results** toolbar, click  **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Parametric Extrusion 1D 1 - Global model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Parametric Extrusion 1D 1**.

Surface 1

1 Right-click **Parametric Extrusion 1D 1 - Global model** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `Hk_Si_bulk`.

4 From the **Unit** list, choose **Å**.

Height Expression 1

1 Right-click **Surface 1** and choose **Height Expression**.

Add the physics interfaces necessary for the space-dependent simulations.

ADD PHYSICS

1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Global model**.

5 Click **Add to Component 1** in the window toolbar.

6 In the tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.

7 In the table, clear the **Solve** check box for **Global model**.

8 Click **Add to Component 1** in the window toolbar.

9 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

HEAVY SPECIES TRANSPORT (HS)

Change the Diffusion Model to Mixture-averaged for the space dependent simulations.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Heavy Species Transport (hs)**.

2 In the **Settings** window for **Heavy Species Transport**, locate the **Diffusion Model** section.

3 From the **Diffusion model** list, choose **Mixture-averaged**.

4 Locate the **Transport Settings** section. Find the **Include** subsection. Select the **Calculate thermodynamic properties** check box.

5 Clear the **Migration in electric field** check box.

6 Select the **Convection** check box.

2: SiH(s)=>Si(s)+0.5H2

1 In the **Model Builder** window, under **Component 1 (comp1)>Heavy Species Transport (hs)** click **2: SiH(s)=>Si(s)+0.5H2**.

2 In the **Settings** window for **Surface Reaction**, locate the **Reaction Formula** section.

3 From the **Specify reaction using** list, choose **Rate coefficient**.

Heavy Species Model 1

1 In the **Model Builder** window, click **Heavy Species Model 1**.

2 In the **Settings** window for **Heavy Species Model**, locate the **Model Inputs** section.

3 From the T list, choose **Temperature (ht)**.

4 From the p_A list, choose **Absolute pressure (spf)**.

5 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

LAMINAR FLOW (SPF)

Since the density variation is not small, the flow cannot be regarded as incompressible. Therefore set the flow to be compressible.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Define the pressure reference level in the interface properties.

4 In the p_{ref} text field, type `13.3[Pa]`.

5 Click the **Show More Options** button in the **Model Builder** toolbar.

6 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Stabilization**.

7 In the tree, select the check box for the node **Physics>Advanced Physics Options**.

8 Click **OK**.

9 In the **Model Builder** window, click **Laminar Flow (spf)**.

10 In the **Settings** window for **Laminar Flow**, click to expand the **Consistent Stabilization** section.

11 Find the **Navier-Stokes equations** subsection. Clear the **Crosswind diffusion** check box.

12 Click to expand the **Discretization** section. From the **Discretization of fluids** list, choose **P2+P1**.

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Laminar Flow (spf)** click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.

3 From the ρ list, choose **Density (hs/cdm1)**.

4 From the μ list, choose **Dynamic viscosity (hs/cdm1)**.

Wall 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Wall**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Wall**, click to expand the **Wall Movement** section.

4 From the **Translational velocity** list, choose **Manual**.

5 Specify the $\mathbf{u}_{tr}$ vector as

hs.mfin/spf.rho	y

6 Click to expand the **Constraint Settings** section. From the **Constraint** list, choose **Nitsche constraints**.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Heat Convection** section.

3 From the **u** list, choose **Velocity field (spf)**.

4 Locate the **Heat Conduction, Fluid** section. From the k list, choose **Thermal conductivity (hs/cdm1)**.

5 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Ideal gas**.

6 From the **Gas constant type** list, choose **Mean molar mass**.

7 From the M_n list, choose **Mean molar mass (hs/cdm1)**.

8 From the C_p list, choose **Heat capacity at constant pressure (hs/cdm1)**.

Temperature 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 In the **Settings** window for **Temperature**, locate the **Temperature** section.

3 In the T_0 text field, type 300.

4 Select Boundaries 1, 3, and 6 only.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type 300.

Boundary Heat Source 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Boundary Heat Source**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Boundary Heat Source**, locate the **Boundary Heat Source** section.

4 From the Q_b list, choose **Total surface heat source of reaction (hs)**.

MESH 1

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 3 and 4 only.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

6 Click the **Custom** button.

7 Locate the **Element Size Parameters** section.

8 Select the **Maximum element size** check box. In the associated text field, type `0.0002`.

Edge 1

1 In the **Mesh** toolbar, click  **Edge**.

2 Select Boundary 4 only.

Size 1

1 Right-click **Edge 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

Free Triangular 1

1 In the **Mesh** toolbar, click  **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click  **Build All**.

ADD STUDY

1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

Add a new study to perform the space dependent simulations.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Output times** text field, type `range(0,5,300)`.

3 In the **Model Builder** window, click **Study 2**.

4 In the **Settings** window for **Study**, type `Space dependent model` in the **Label** text field.

Solution 2 (sol2)

1 In the **Study** toolbar, click  **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.

3 In the **Model Builder** window, under **Space dependent model>Solver Configurations>Solution 2 (sol2)** click **Time-Dependent Solver 1**.

4 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute Tolerance** section.

5 From the **Global method** list, choose **Unscaled**.

6 Click to expand the **Time Stepping** section. In the **Initial step** text field, type `0.001`.

7 Click **Compute**.

RESULTS

Velocity (spf)

1 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

2 From the **Time (s)** list, choose **5**.

Surface

1 In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `v`.

4 In the **Velocity (spf)** toolbar, click **Plot**.

Temperature (ht)

1 In the **Model Builder** window, under **Results** click **Temperature (ht)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **5**.

Surface

1 In the **Model Builder** window, expand the **Temperature (ht)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `T-300[K]`.

4 In the **Temperature (ht)** toolbar, click **Plot**.

Diffusion Velocity, Hydrogen

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Diffusion Velocity, Hydrogen` in the **Label** text field.

3 Locate the **Data** section. From the **Time (s)** list, choose **5**.

4 From the **Dataset** list, choose **Space dependent model/Solution 2 (sol2)**.

Surface 1

1 Right-click **Diffusion Velocity, Hydrogen** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `hs.Vdy_wH2`.

4 In the **Diffusion Velocity, Hydrogen** toolbar, click **Plot**.

Plot the global model and space dependent simulation together.

Average Pressure Divided by Average Initial Pressure

1 In the **Model Builder** window, under **Results** click **Average Pressure Divided by Average Initial Pressure**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `Average pressure divided by average initial pressure`.

Space dependent model

1 Right-click **Average Pressure Divided by Average Initial Pressure** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`intop1(spf.pA)/at(0,intop1(spf.pA))`	1	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Space dependent model`

7 In the **Average Pressure Divided by Average Initial Pressure** toolbar, click **Plot**.

Density ratio

1 In the **Model Builder** window, under **Results** click **Density ratio**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** check box. In the associated text field, type `Initial mass divided by the mass in the reactor`.

Space dependent model

1 Right-click **Density ratio** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`at(0,intop1(hs.rho))/intop1(hs.rho)`	1	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Space dependent model`

7 In the **Density ratio** toolbar, click **Plot**.

Total Reactor Mass

1 In the **Model Builder** window, under **Results** click **Total Reactor Mass**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** check box. In the associated text field, type `Mass density (kg/m)`.

Space dependent model

1 Right-click **Total Reactor Mass** and choose **Global**.

2 In the **Settings** window for **Global**, type `Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Space dependent model/ Solution 2 (sol2)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`mass_domain`	`kg/m`	`Mass change in the domain`
`mass_surf+mass_bulk`	`kg/m`	

5 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`mass_domain: Space dependent model`
`mass_surf+mass_bulk: Space dependent model`

7 In the **Total Reactor Mass** toolbar, click **Plot**.

Plot the Si growth height computed with the space dependent model.

Edge 2D 2

1 In the **Results** toolbar, click **More Datasets** and choose **Edge 2D**.

2 In the **Settings** window for **Edge 2D**, locate the **Data** section.

3 From the **Dataset** list, choose **Space dependent model/Solution 2 (sol2)**.

4 Select Boundary 4 only.

Parametric Extrusion 1D 2

1 In the **Results** toolbar, click **More Datasets** and choose **Parametric Extrusion 1D**.

2 In the **Settings** window for **Parametric Extrusion 1D**, locate the **Data** section.

3 From the **Dataset** list, choose **Edge 2D 2**.

Parametric Extrusion 1D 1 - Space dependent model

1 In the **Model Builder** window, right-click **Parametric Extrusion 1D 1 - Global model** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Parametric Extrusion 1D 1 - Space dependent model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Parametric Extrusion 1D 2**.

4 In the **Parametric Extrusion 1D 1 - Space dependent model** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.