



Model created in COMSOL Multiphysics 6.4

Chemical Vapor Deposition of Titanium Nitride on Machining Tool Inserts

Introduction

Chemical vapor deposition (CVD) is a process used to grow thin films on substrates. In this CVD example, metal inserts for machining tools are coated with titanium nitride (TiN). The titanium nitride layer improves the wear resistance of the metal inserts by increasing the hardness, reducing friction, and reducing oxidation. Additionally, due to its golden appearance, the coating process is also performed for aesthetic purposes. The CVD reactor in this example operates at low pressures and high temperatures. These operating conditions ensure high diffusion, which is needed for efficient mass transfer onto the substrate surfaces and for homogeneous deposition thicknesses (Ref. 1).

Model Definition

This model describes the coupled reaction kinetics, fluid flow, and mass transfer in the CVD reactor. The temperature is assumed to be held constant at 1100 K.

MODEL GEOMETRY

The CVD reactor used in this coating process is made up of vertically stacked trays where each tray contains the metal inserts to be coated. [Figure 1](#) illustrates one of these reactor trays where gas is fed from the center, reacts on the metal insert surfaces, and exits through the outer reactor wall.

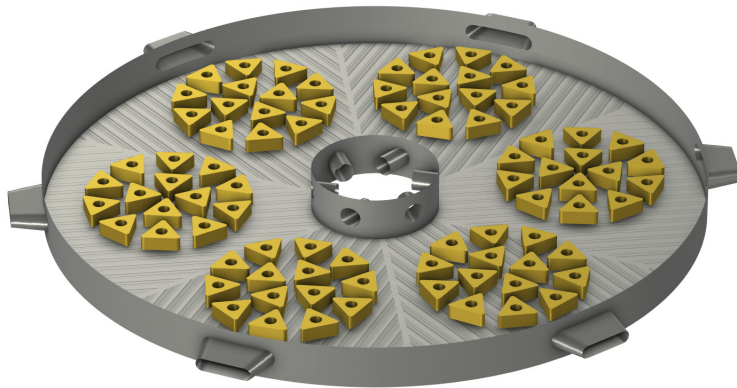


Figure 1: Chemical vapor deposition reactor tray design used in this example.

Figure 2 shows the modeled domain which consists of a sixth of the full reactor tray shown in Figure 1 above. This simplification is made due to the symmetry of the reactor in order to reduce the computational time.

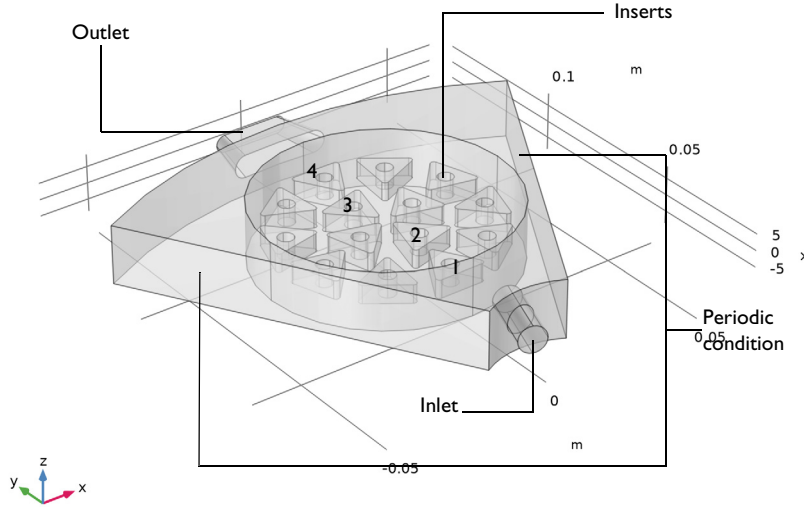
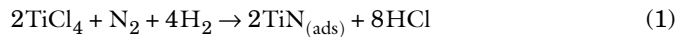


Figure 2: Model geometry including the domain and boundary labels. The labeled inserts (1 through 4) refer to the inserts that are studied in the Results and Discussion section.

CHEMISTRY

The gas phase titanium chloride (TiCl_4) reacts with nitrogen (N_2) to form solid phase titanium nitride (TiN) on the surface of the metal insert based on the following reaction:



The deposition rate ($\text{mol}/(\text{m}^2 \cdot \text{s})$) of TiN on the metal substrates is defined according to Popovska and others as follows (Ref. 1):

$$r = k \cdot p_{\text{TiCl}_4}^{5/4} \cdot \sqrt{p_{\text{H}_2} p_{\text{N}_2}} \quad (2)$$

where p_i is the nondimensional partial pressure of species i and k is the partially nondimensional rate constant ($\text{mol}/(\text{m}^2 \cdot \text{s})$) with reference pressure 1 Pa. The rate constant is described by the Arrhenius expression as follows:

$$k = A \exp\left(-\frac{E}{RT}\right) \quad (3)$$

where A is the partially nondimensional Arrhenius constant, 6.51×10^{16} mol/(m²·s) with reference pressure 1 Pa, and E is the activation energy, 7×10^3 J/mol (Ref. 1).

FLUID FLOW

The fluid flow of the gas phase is described by the Navier–Stokes equations and is modeled assuming weakly compressible, laminar flow. The inlet of the gas has a normal mass flow rate boundary condition and the outlet of the gas has a pressure boundary condition where no backflow is enforced. Periodic flow boundary conditions are applied on the sides of the modeled geometry and there is no pressure drop across these boundaries.

MASS TRANSFER

As seen in the chemical reaction (Equation 1), there are 5 species involved in the heterogeneous chemical reaction for the deposition process, four of which are gaseous species (TiCl₄, N₂, H₂, and HCl) and one of which is a surface species (TiN).

The Transport of Concentrated Species interface is used to describe the mass transfer in the gas phase and is defined on all domains. This interface is used because there is no clear solvent choice, given the comparable amounts of the involved species, and because the gas density varies due to material removal during the adsorption reaction. The mass flux in the system consists of convective and diffusive flux. The diffusive flux is described with the mixture-averaged diffusion model. The gas inflow boundary condition is defined from a mole fraction. The surface reaction is modeled with a general inward flux boundary condition which is defined on the surface of the metal inserts as follows:

$$j_i = M_i R_i \quad (4)$$

where j_i is the mass flux (kg/(m²·s)), M_i is the molar mass (kg/mol), and R_i is the surface reaction rate (mol/(m²·s)) based on Equation 2 for species i ($i = \text{TiCl}_4, \text{N}_2, \text{H}_2, \text{HCl}$). In an analogous manner to the fluid flow description, periodic condition boundaries are applied to the sides of the domain for mass transfer.

The Surface Reactions interface is used to describe the mass transfer in the adsorbed phase and is defined only on the surface of the metal inserts. The reaction rate for the surface species, TiN, is defined from Equation 2 (mol/(m²·s)). This interface is only enabled in the time-second study to solve for the time evolution of the deposition thickness.

COMPUTATION

Two studies are computed in order to better understand how the mass flow rate affects the deposition rates, and how the position of tools within the tray affects deposition thickness:

- 1 A stationary study is solved to investigate how varying the inlet gas mass flow rate affects the deposition rate across the metal tools. This study is achieved by using an auxiliary sweep to vary the total inlet mass flow rate by factors of 1/5, 1/2, 1, 2, and 5.
- 2 A time-dependent study is solved to investigate how rotating the tools within the tray affects the evenness of the deposition thickness layer. This study is achieved by using a rotating domain with a moving mesh in order to ensure each tool spends an equal amount of time at each position.

Results and Discussion

Figure 3 below shows the deposition rate of TiN on the metal insert surfaces. The deposition rate on the surface of the metal inserts is the highest near the gas inlet and decreases over the distance where the reactants are consumed.

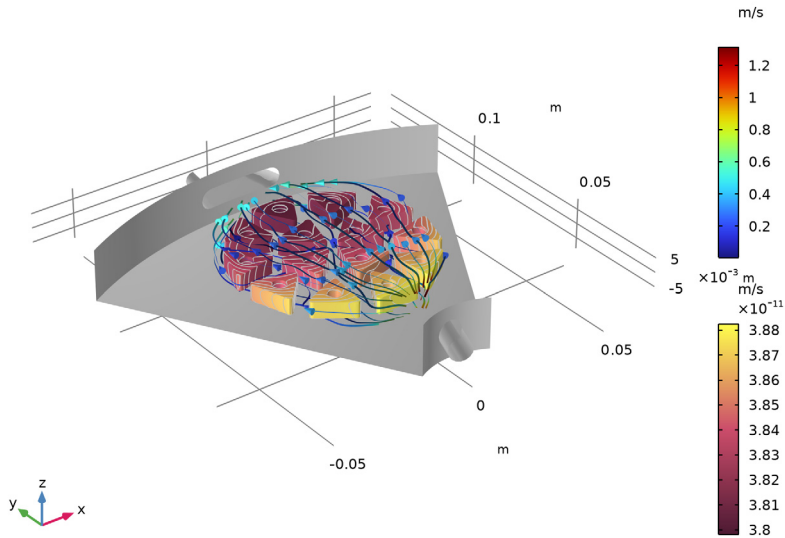


Figure 3: TiN deposition rate (m/s) on the metal insert surface and gas velocity field (m/s) streamlines for the mass flow rate base case ($mfac = 1$).

Figure 4 and Figure 5 show the deposition rate on four inserts and the variation between the homogeneity of the deposition rate. In both figures, the x -axis (mfac) refers to a factor of the base case inlet flow rate, 3.3×10^{-6} kg/s. The inserts 1 through 4 that are studied are indicated on the model domain geometry shown in Figure 2.

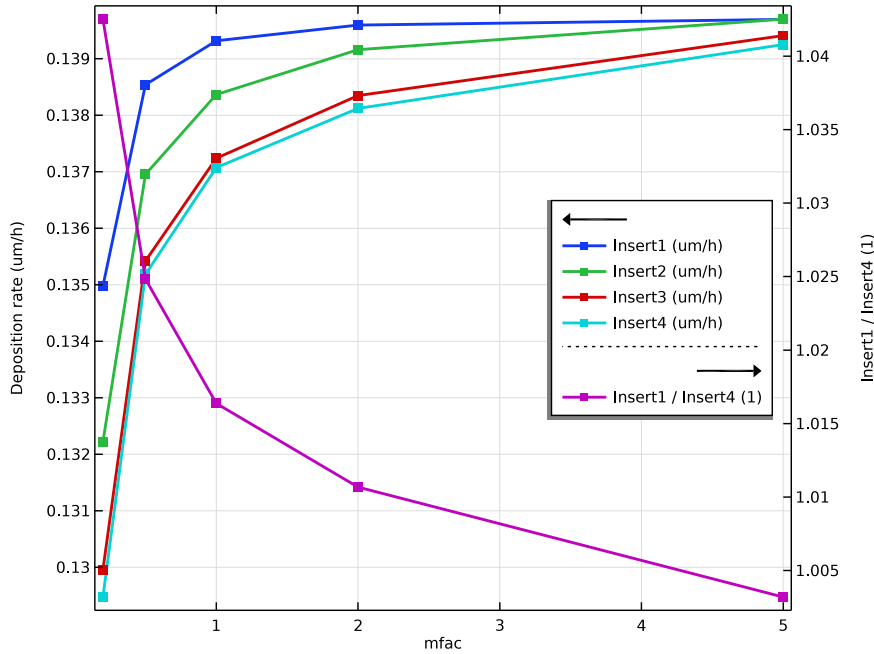


Figure 4: Average deposition rates for inserts 1 through 4 (m/h) and deposition rate homogeneity factor as a function of the inlet flow rate. The x -axis 'mfac' represents a factor of the base-case inlet flow rate, $3.3 \cdot 10^{-6}$ kg/s.

Figure 4 shows that the metal insert located closest to the gas inlet (insert 1) has the highest deposition rate, whereas the metal insert located furthest from the gas inlet (insert 4) has the lowest deposition rate. This trend is due to the higher TiCl_4 concentrations near the feed. Figure 4 also shows that higher total inlet mass flow rates result in higher depositions rate and also more uniform deposition rates between the metal insert locations in the tray.

Figure 5 shows another approach to comparing the homogeneity of the deposition by comparing the variation in the deposition rate.

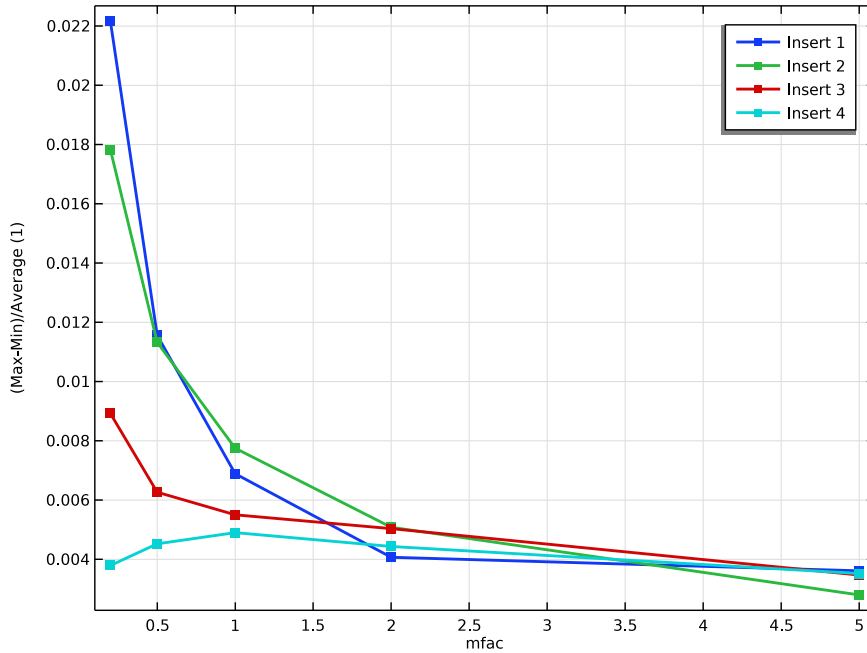


Figure 5: Variation between the deposition rates for inserts 1 through 4.

Figure 5 clearly shows that, as the mass flow rate increases, there is less variation in the deposition rates across the insert surfaces.

Based on the trends shown in Figure 4 and Figure 5, a mass flow rate factor of 1, corresponding to an inlet flow rate of 3.3×10^{-6} kg/s, represents a good compromise between uniform deposition rates and efficient use of the injected gas feed. Therefore, this value is used in the second time-dependent study.

Figure 6 shows the deposition layer thickness for the metal inserts and the relative difference between insert 1 and insert 4 for the rotating insert section study.

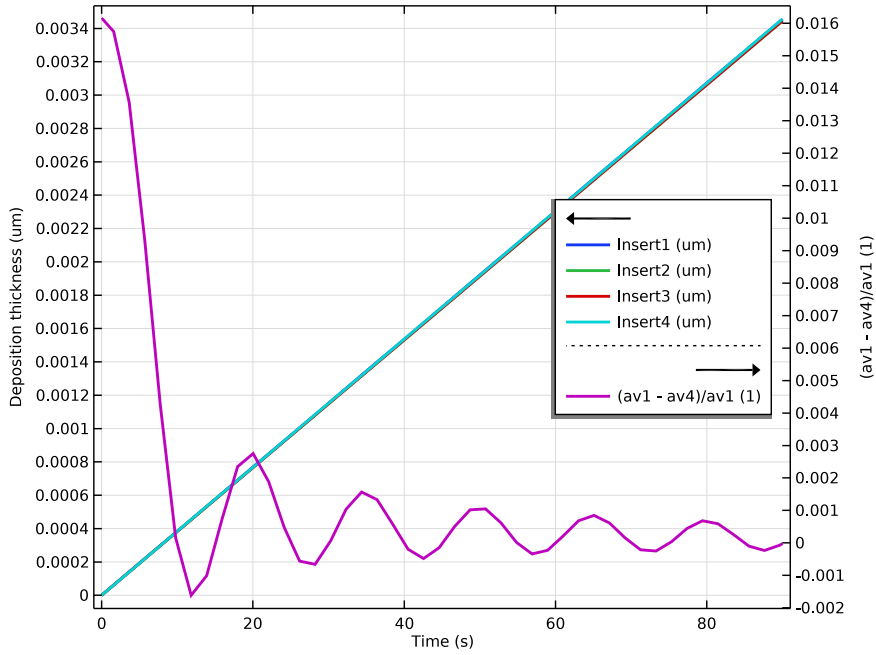


Figure 6: Deposition layer thickness for inserts 1 through 4 (m) and the relative difference in thickness between insert 1 and insert 4 over time.

Figure 6 shows that the deposition layer thickness is rather uniform between the four inserts studied over time. Initially, the relative deposition thickness difference between insert 1 and insert 4 is approximately 1.6%. This value decreases in an oscillatory manner due to the rotation of the metal inserts until the relative difference is nearly negligible after 90 s. These results show that the rotation results in a more uniform TiN coating thickness across all of the metal tools, compared to what is expected from the nonrotating (stationary) case.

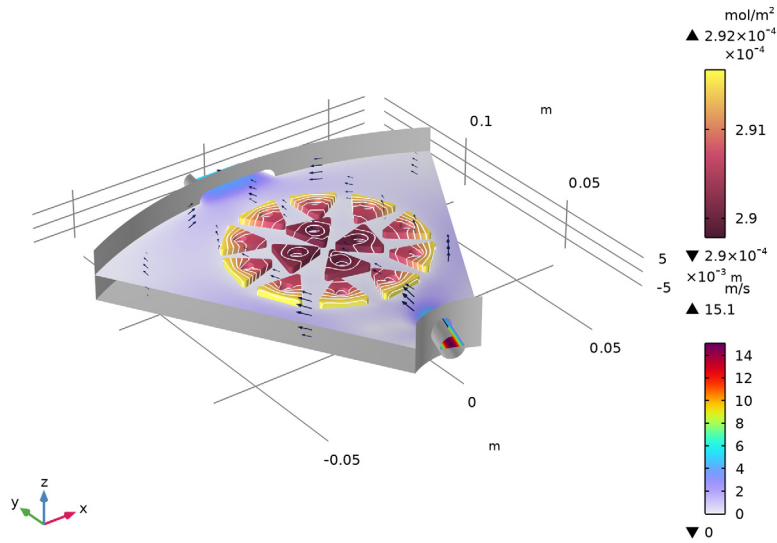


Figure 7: TiN surface concentration (mol/m^2) with contour plots showing the deposition thickness (m), the gas velocity (m/s) with arrows for the velocity field, and results at 90 s.

Figure 7 shows how the surface concentration of TiN on the metal inserts decreases toward the center of the subdomain containing the metal inserts due to the decrease in TiCl_4 in the gas phase as the reaction progresses.

Reference


I. N. Popovska, S. Poscher, P. Tichy, G. Emig, and H. Ryssel, “Kinetics of Chemical Vapor Deposition of Titanium Nitride,” *Electrochemical Society Proceedings*, vol. 97, no. 25, pp. 592–596, 1997.

Application Library path: Chemical_Reaction_Engineering_Module/
Reactors_with_Mass_Transfer/TiN_cvd_reactor


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  **3D**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport > Chemistry (chem)**.
- 3 Click **Add**.
- 4 In the **Select Physics** tree, select **Chemical Species Transport > Transport of Concentrated Species (tcs)**.
- 5 Click **Add**.
- 6 In the **Number of species** text field, type 4.
- 7 In the **Mass fractions (I)** table, enter the following settings:

wH2



wN2

wTiCl4

wHCl


- 8 In the **Select Physics** tree, select **Chemical Species Transport > Surface Reactions (sr)**.
- 9 Click **Add**.
- 10 In the **Surface (adsorbed) species concentrations (mol/m²)** table, enter the following settings:

cTiN



- 11 In the **Select Physics** tree, select **Fluid Flow > Single-Phase Flow > Laminar Flow (spf)**.
- 12 Click **Add**.
- 13 Click  **Study**.
- 14 In the **Select Study** tree, select **General Studies > Stationary**.
- 15 Click  **Done**.

GLOBAL DEFINITIONS



Geometry Parameters

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 2 In the **Settings** window for **Parameters**, type Geometry Parameters in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `TiN_cvd_reactor_geom_parameters.txt`.

Process Parameters


- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Process Parameters in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `TiN_cvd_reactor_process_parameters.txt`.

Physical Parameters

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Physical Parameters in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `TiN_cvd_reactor_physical_parameters.txt`.

GEOMETRY I


Work Plane 1 (wp1)

- 1 In the **Geometry** toolbar, click  **Work Plane**.
- 2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.
- 3 In the **z-coordinate** text field, type $-H/2$.
- 4 Locate the **Unite Objects** section. Clear the **Unite objects** checkbox.

Work Plane 1 (wp1) > Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.



Work Plane 1 (wp1) > Circle 1 (c1)

- 1 In the **Work Plane** toolbar, click  **Circle**.
- 2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type rReactorIn.
- 4 In the **Sector angle** text field, type 360/sectors.
- 5 Locate the **Rotation Angle** section. In the **Rotation** text field, type 90-360/sectors/2.


Work Plane 1 (wp1) > Circle 2 (c2)

- 1 Right-click **Component 1 (comp1) > Geometry 1 > Work Plane 1 (wp1) > Plane Geometry > Circle 1 (c1)** and choose **Duplicate**.
- 2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type rReactorOut.




Work Plane 1 (wp1) > Difference 1 (dif1)

- 1 In the **Work Plane** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **c2** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 5 Select the object **c1** only.

Work Plane 1 (wp1) > Circle 3 (c3)

- 1 In the **Work Plane** toolbar, click  **Circle**.
- 2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type rRotating.
- 4 Locate the **Position** section. In the **yw** text field, type rRotatingCenter.

Work Plane 1 (wp1) > Difference 2 (dif2)


- 1 In the **Work Plane** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **dif1** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 5 Select the object **c3** only.
- 6 Select the **Keep objects to subtract** checkbox.
- 7 In the **Work Plane** toolbar, click  **Build All**.

Extrude 1 (ext1)


- 1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.
- 2 In the **Settings** window for **Extrude**, locate the **General** section.
- 3 From the **Extrude from** list, choose **Faces**.
- 4 On the object **wp1.dif2**, select Boundary 1 only.
- 5 On the object **wp1.c3**, select Boundary 1 only.
- 6 Locate the **Distances** section. In the table, enter the following settings:

| Distances (m) |
|----------------------|
| H |


Cylinder 1 (cyl1)

- 1 In the **Geometry** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type r_{Injector} .
- 4 In the **Height** text field, type $5 * r_{\text{Injector}}$.
- 5 Locate the **Position** section. In the **y** text field, type $0.6 * r_{\text{ReactorIn}}$.
- 6 Locate the **Axis** section. From the **Axis type** list, choose **y-axis**.
- 7 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

Rotate 1 (rot1)

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Rotate**.
- 2 Select the object **cyl1** only.
- 3 In the **Settings** window for **Rotate**, locate the **Rotation** section.
- 4 In the **Angle** text field, type -20.
- 5 Locate the **Point on Axis of Rotation** section. In the **y** text field, type $r_{\text{ReactorIn}}$.


Work Plane 2 (wp2)

- 1 In the **Geometry** toolbar, click  **Work Plane**.
- 2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.
- 3 From the **Plane** list, choose **xz-plane**.
- 4 In the **y-coordinate** text field, type $r_{\text{ReactorOut}} * 0.985$.



Work Plane 2 (wp2) > Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 2 (wp2) > Rectangle 1 (r1)

- 1 In the **Work Plane** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type Wextractor.
- 4 In the **Height** text field, type Hextractor.
- 5 Locate the **Position** section. From the **Base** list, choose **Center**.

Work Plane 2 (wp2) > Fillet 1 (fil1)

- 1 In the **Work Plane** toolbar, click  **Fillet**.
- 2 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 3 On the object **r1**, select Points 1–4 only.
- 4 In the **Settings** window for **Fillet**, locate the **Radius** section.
- 5 In the **Radius** text field, type Hextractor*0.5.

Extrude 2 (ext2)



- 1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.
- 2 In the **Settings** window for **Extrude**, locate the **Distances** section.
- 3 In the table, enter the following settings:

| Distances (m) |
|----------------------|
| -Wextractor/2 |

- 4 Click to expand the **Scales** section. In the table, enter the following settings:

| Scales xw | Scales yw |
|------------------|------------------|
| 0.75 | 0.75 |


Difference 1 (dif1)

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **ext2** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 5 Select the objects **ext1(1)** and **ext1(2)** only.
- 6 Select the **Keep objects to subtract** checkbox.
- 7 Clear the **Keep interior boundaries** checkbox.

Union 1 (uni1)

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Union**.
- 2 Select the objects **dif1**, **ext1(I)**, and **rot1** only.


Work Plane 3 (wp3)

- 1 In the **Geometry** toolbar, click  **Work Plane**.
- 2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.
- 3 In the **z-coordinate** text field, type $-H/2+H_{insert}$.

Work Plane 3 (wp3) > Plane Geometry


In the **Model Builder** window, click **Plane Geometry**.

Work Plane 3 (wp3) > Polygon 1 (pol1)



- 1 In the **Work Plane** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
- 3 In the table, enter the following settings:

| xw (m) | yw (m) |
|---------------------|-------------------------------------|
| 0 | 0 |
| $L_{insert} * 0.5$ | $L_{insert} * \cos(30[\text{deg}])$ |
| $-L_{insert} * 0.5$ | $L_{insert} * \cos(30[\text{deg}])$ |
| 0 | 0 |



Work Plane 3 (wp3) > Circle 1 (c1)

- 1 In the **Work Plane** toolbar, click  **Circle**.
- 2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.
- 3 In the **Radius** text field, type $L_{insert}/7$.
- 4 Locate the **Position** section. In the **yw** text field, type $L_{insert} * (1 - \cos(30[\text{deg}])) * 0.5$.


Work Plane 3 (wp3) > Difference 1 (dif1)

- 1 In the **Work Plane** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **pol1** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 5 Select the object **c1** only.


Work Plane 3 (wp3) > Fillet 1 (fil1)

- 1 In the **Work Plane** toolbar, click  **Fillet**.
- 2 In the **Settings** window for **Fillet**, locate the **Points** section.
- 3 Click to select the  **Activate Selection** toggle button for **Vertices to fillet**.
- 4 On the object **dif1**, select Points 1, 3, and 7 only.
- 5 Locate the **Radius** section. In the **Radius** text field, type 1.0[mm].


Work Plane 3 (wp3) > Move 1 (mov1)

- 1 In the **Work Plane** toolbar, click  **Transforms** and choose **Move**.
- 2 Select the object **fill** only.
- 3 In the **Settings** window for **Move**, locate the **Displacement** section.
- 4 In the **yw** text field, type rRotatingCenter+rRotating*0.49.


Work Plane 3 (wp3) > Rotate 1 (rot1)

- 1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.
- 2 Select the object **mov1** only.
- 3 In the **Settings** window for **Rotate**, locate the **Input** section.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Rotation** section. In the **Angle** text field, type 36.
- 6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Rotate 2 (rot2)

- 1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.
- 2 Click in the **Graphics** window and then press Ctrl+A to select both objects.
- 3 In the **Settings** window for **Rotate**, locate the **Input** section.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Rotation** section. In the **Angle** text field, type 72.
- 6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Rotate 3 (rot3)

- 1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.
- 2 Click in the **Graphics** window and then press Ctrl+A to select all objects.
- 3 In the **Settings** window for **Rotate**, locate the **Input** section.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Rotation** section. In the **Angle** text field, type 144.

6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Copy 1 (copy1)


1 In the **Work Plane** toolbar, click  **Transforms** and choose **Copy**.

2 Select the object **mov1** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **yw** text field, type -Linsert*1.00.

Work Plane 3 (wp3) > Rotate 4 (rot4)

1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.


2 Select the object **copy1** only.

3 In the **Settings** window for **Rotate**, locate the **Rotation** section.

4 In the **Angle** text field, type 15.

5 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Rotate 5 (rot5)

1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.

2 Select the object **rot4** only.

3 In the **Settings** window for **Rotate**, locate the **Input** section.

4 Select the **Keep input objects** checkbox.

5 Locate the **Rotation** section. In the **Angle** text field, type 90.

6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Rotate 6 (rot6)

1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.

2 Select the objects **rot4** and **rot5** only.


3 In the **Settings** window for **Rotate**, locate the **Input** section.

4 Select the **Keep input objects** checkbox.

5 Locate the **Rotation** section. In the **Angle** text field, type 180.

6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.

Work Plane 3 (wp3) > Rotate 7 (rot7)

1 In the **Work Plane** toolbar, click  **Transforms** and choose **Rotate**.

2 Select the objects **mov1**, **rot1**, **rot2(1)**, **rot2(2)**, **rot3(1)**, **rot3(2)**, **rot3(3)**, and **rot3(4)** only.

3 In the **Settings** window for **Rotate**, locate the **Input** section.

4 Select the **Keep input objects** checkbox.

- 5 Locate the **Rotation** section. In the **Angle** text field, type 72+36.
- 6 Locate the **Center of Rotation** section. In the **yw** text field, type rRotatingCenter.




Extrude 3 (ext3)

- 1 In the **Model Builder** window, right-click **Geometry 1** and choose **Extrude**.
- 2 In the **Settings** window for **Extrude**, locate the **Distances** section.
- 3 In the table, enter the following settings:

| Distances (m) |
|----------------------|
| Hinsert |

- 4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.
- 5 From the **Show in physics** list, choose **All levels**.


Difference 2 (dif2)

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **ext1(2)** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.
- 5 Click the  **Paste Selection** button for **Objects to subtract**.
- 6 In the **Paste Selection** dialog, type ext3 in the **Selection** text field.
- 7 Click **OK**.

Form Assembly

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Geometry 1** click **Form Union (fin)**.
- 2 In the **Settings** window for **Form Union/Assembly**, type Form Assembly in the **Label** text field.
- 3 Locate the **Form Union/Assembly** section. From the **Action** list, choose **Form an assembly**.

Ignore Faces 1 (igf1)

- 1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Ignore Faces**.
- 2 On the object **fin**, select Boundary 9 only.

Cumulative Selections

In the **Geometry** toolbar, click  **Selections** and choose **Cumulative Selections**.

Inserts

- 1 Right-click **Cumulative Selections** and choose **Cumulative Selection**.
- 2 In the **Settings** window for **Selection**, type **Inserts** in the **Label** text field.


Injector

- 1 In the **Model Builder** window, right-click **Cumulative Selections** and choose **Cumulative Selection**.
- 2 In the **Settings** window for **Selection**, type **Injector** in the **Label** text field.

Cylinder 1 (cyl1)


- 1 In the **Model Builder** window, under **Component 1 (comp1) > Geometry 1** click **Cylinder 1 (cyl1)**.
- 2 In the **Settings** window for **Cylinder**, locate the **Selections of Resulting Entities** section.
- 3 Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Injector**.

Extrude 3 (ext3)

- 1 In the **Model Builder** window, click **Extrude 3 (ext3)**.
- 2 In the **Settings** window for **Extrude**, locate the **Selections of Resulting Entities** section.
- 3 Find the **Cumulative selection** subsection. From the **Contribute to** list, choose **Inserts**.
- 4 In the **Geometry** toolbar, click  **Build All**.


DEFINITIONS

Variables 1


- 1 In the **Model Builder** window, expand the **Component 1 (comp1) > Definitions** node.
- 2 Right-click **Definitions** and choose **Variables**.
- 3 In the **Settings** window for **Variables**, locate the **Variables** section.
- 4 Click  **Load from File**.
- 5 Browse to the model's Application Libraries folder and double-click the file `TiN_cvd_reactor_variables.txt`.

Insert Boundary Variables


- 1 Right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type **Insert Boundary Variables** in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

- 4 From the **Selection** list, choose **Inserts**.
- 5 Locate the **Variables** section. Click  **Load from File**.
- 6 Browse to the model's Application Libraries folder and double-click the file `TiN_cvd_reactor_insert_boundary_variables.txt`.


Step 1 (step1)

- 1 In the **Definitions** toolbar, click  **More Functions** and choose **Step**.
- 2 In the **Settings** window for **Step**, click to expand the **Smoothing** section.
- 3 In the **Size of transition zone** text field, type `t_rot`.


Inlet

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type `Inlet` in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 15 only.


Outlet

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type `Outlet` in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundary 10 only.



Rotating Domain

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type `Rotating Domain` in the **Label** text field.
- 3 Select Domain 4 only.



Inserts Vertical Bnds

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type `Inserts Vertical Bnds` in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type `0.99*rRotating`.
- 5 In the **Top distance** text field, type `0.25*Hinsert`.
- 6 In the **Bottom distance** text field, type `-0.25*Hinsert`.
- 7 Locate the **Position** section. In the **y** text field, type `rRotatingCenter`.


Insert Horizontal Edges

- 1 In the **Definitions** toolbar, click  **Adjacent**.
- 2 In the **Settings** window for **Adjacent**, type Insert Horizontal Edges in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Under **Input selections**, click  **Add**.
- 5 In the **Add** dialog, select **Inserts Vertical Bnds** in the **Input selections** list.
- 6 Click **OK**.
- 7 In the **Settings** window for **Adjacent**, locate the **Output Entities** section.
- 8 From the **Geometric entity level** list, choose **Adjacent edges**.


Insert Vertical Edges

- 1 In the **Definitions** toolbar, click  **Adjacent**.
- 2 In the **Settings** window for **Adjacent**, type Insert Vertical Edges in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Under **Input selections**, click  **Add**.
- 5 In the **Add** dialog, select **Inserts Vertical Bnds** in the **Input selections** list.
- 6 Click **OK**.
- 7 In the **Settings** window for **Adjacent**, locate the **Output Entities** section.
- 8 From the **Geometric entity level** list, choose **Adjacent edges**.
- 9 From the **Exterior edges** list, choose **None**.
- 10 Select the **Interior edges** checkbox.



Insert Top Bnds

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert Top Bnds in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type $0.99 * r_{Rotating}$.
- 5 In the **Top distance** text field, type H_{insert} .
- 6 In the **Bottom distance** text field, type $0[mm]$.
- 7 Locate the **Position** section. In the **y** text field, type $r_{RotatingCenter}$.
- 8 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.


Insert Bottom Bnds

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert Bottom Bnds in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type 0.036.
- 5 In the **Top distance** text field, type 0[mm].
- 6 In the **Bottom distance** text field, type -4[mm].
- 7 Locate the **Position** section. In the **y** text field, type rRotatingCenter.
- 8 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.


Sliding Mesh, Source Bnds

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Sliding Mesh, Source Bnds in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 5, 6, 24, and 25 only.
- 5 Click the  **Zoom to Selection** button in the **Graphics** toolbar.


Sliding Mesh Destination Bnds

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Sliding Mesh Destination Bnds in the **Label** text field.
- 3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 29, 30, 125, and 130 only.


Insert I

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert I in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type Linsert*0.6.
- 5 Locate the **Position** section. In the **y** text field, type rRotatingCenter - (3/4)* rRotating.
- 6 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.




Insert 2

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert 2 in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type $L_{\text{insert}} * 0.6$.
- 5 Locate the **Position** section. In the **x** text field, type $L_{\text{insert}} * 0.15$.
- 6 In the **y** text field, type $r_{\text{RotatingCenter}} - (1/4) * r_{\text{Rotating}}$.
- 7 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.

Insert 3


- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert 3 in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type $L_{\text{insert}} * 0.6$.
- 5 Locate the **Position** section. In the **x** text field, type $-L_{\text{insert}} * 0.15$.
- 6 In the **y** text field, type $r_{\text{RotatingCenter}} + (1/4) * r_{\text{Rotating}}$.
- 7 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.

Insert 4

- 1 In the **Definitions** toolbar, click  **Cylinder**.
- 2 In the **Settings** window for **Cylinder**, type Insert 4 in the **Label** text field.
- 3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.
- 4 Locate the **Size and Shape** section. In the **Outer radius** text field, type $L_{\text{insert}} * 0.6$.
- 5 Locate the **Position** section. In the **y** text field, type $r_{\text{RotatingCenter}} + (3/4) * r_{\text{Rotating}}$.
- 6 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside cylinder**.
- 7 Click the  **Show More Options** button in the **Model Builder** toolbar.
- 8 In the **Show More Options** dialog, select **Physics > Advanced Physics Options** in the tree.
- 9 In the tree, select the checkbox for the node **Physics > Advanced Physics Options**.
- 10 Click **OK**.
- 11 Click the  **Zoom Extents** button in the **Graphics** toolbar.

COMPONENT 1 (COMP1)


Rotating Domain 1

- 1 In the **Physics** toolbar, click  **Moving Mesh** and choose **Rotating Domain**.
- 2 In the **Settings** window for **Rotating Domain**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Rotating Domain**.
- 4 Locate the **Rotation** section. From the **Rotation type** list, choose **Specified rotational velocity**.
- 5 From the **Rotational velocity expression** list, choose **General revolutions per time**.
- 6 In the f text field, type $\text{rpm} * \text{step1}(t)$.
- 7 Locate the **Axis** section. Specify the \mathbf{r}_{ax} vector as

| | |
|----------------------|---|
| root.rRotatingCenter | Y |
|----------------------|---|


MULTIPHYSICS

Reacting Flow 1 (nirf1)

- 1 In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain > Reacting Flow**.
- 2 In the **Settings** window for **Reacting Flow**, locate the **Coupled Interfaces** section.
- 3 From the **Chemistry (optional)** list, choose **None**.

CHEMISTRY (CHEM)

Reaction 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **Reaction**.
- 2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
- 3 In the **Formula** text field, type $2 \text{ TiCl}_4 + \text{N}_2 + 4 \text{ H}_2 \Rightarrow 2 \text{ TiN}(\text{ads}) + 8 \text{ HCl}$.
- 4 Click **Apply**.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $k_{\text{Pop}} * p_{\text{TiCl}_4}^{1.25} * p_{\text{H}_2}^{0.5} * p_{\text{N}_2}^{0.5}$.
- 7 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 1.
- 8 In the **Model Builder** window, click **Chemistry (chem)**.
- 9 In the **Settings** window for **Chemistry**, locate the **Model Input** section.
- 10 From the T list, choose **User defined**. In the associated text field, type T_{reac} .

- 11 From the p list, choose **User defined**. In the associated text field, type p_{Ref} .
- 12 Locate the **Mixture Properties** section. From the **Type** list, choose **Concentrated species**.
- 13 Locate the **Species Matching** section. Find the **Bulk species** subsection. From the **Species solved for** list, choose **Transport of Concentrated Species**.
- 14 In the table, enter the following settings:

| Species | Type | Mass fraction | Value (I) |
|---------|----------|---------------|------------|
| H2 | Variable | wH2 | Solved for |
| HCl | Variable | wHCl | Solved for |
| N2 | Variable | wN2 | Solved for |
| TiCl4 | Variable | wTiCl4 | Solved for |

- 15 Find the **Surface species** subsection. From the **Species solved for** list, choose **Surface Reactions**.
- 16 In the table, enter the following settings:

| Species | Type | Surface concentration | Value (mol/m ²) |
|----------|----------|-----------------------|-----------------------------|
| TiN(ads) | Variable | cTiN | Solved for |

Species: *TiCl4*

- 1 In the **Model Builder** window, click **Species: TiCl4**.
- 2 In the **Settings** window for **Species**, click to expand the **Transport Expressions** section.
- 3 In the σ text field, type $LJpot_TiCl4$.
- 4 In the ϵ/k_b text field, type $epsilon_k_TiCl4$.

Species: *N2*

- 1 In the **Model Builder** window, click **Species: N2**.
- 2 In the **Settings** window for **Species**, locate the **Transport Expressions** section.
- 3 In the σ text field, type $LJpot_N2$.
- 4 In the ϵ/k_b text field, type $epsilon_k_N2$.

Species: *H2*

- 1 In the **Model Builder** window, click **Species: H2**.
- 2 In the **Settings** window for **Species**, locate the **Transport Expressions** section.
- 3 In the σ text field, type $LJpot_H2$.
- 4 In the ϵ/k_b text field, type $epsilon_k_H2$.

Species: HCl

- 1 In the **Model Builder** window, click **Species: HCl**.
- 2 In the **Settings** window for **Species**, locate the **Transport Expressions** section.
- 3 In the σ text field, type `LJpot_HCl`.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Concentrated Species (tcs)**.

Inflow 1

In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.

Outflow 1

In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.

Flux 1

In the **Physics** toolbar, click  **Boundaries** and choose **Flux**.

Periodic Condition 1

In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Condition**.

Fluid 1

- 1 In the **Model Builder** window, click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Model Input** section.
- 3 From the T list, choose **User defined**. In the associated text field, type `Treac`.
- 4 Locate the **Density** section. From the ρ list, choose **Density (chem)**.
- 5 Locate the **Diffusion** section. In the table, enter the following settings:

| Species 1 | Species 2 | Diffusivity | Diffusion coefficient (m²/s) |
|------------------|------------------|--------------------|--|
| wH2 | wN2 | User defined | <code>chem.D_H2_N2</code> |
| wH2 | wTiCl4 | User defined | <code>chem.D_H2_TiCl4</code> |
| wH2 | wHCl | User defined | <code>chem.D_H2_HCl</code> |
| wN2 | wTiCl4 | User defined | <code>chem.D_N2_TiCl4</code> |
| wN2 | wHCl | User defined | <code>chem.D_N2_HCl</code> |
| wTiCl4 | wHCl | User defined | <code>chem.D_TiCl4_HCl</code> |

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 From the **Mixture specification** list, choose **Mole fractions**.

4 In the x_{0,wN_2} text field, type xN_2in .

5 In the $x_{0,wTiCl_4}$ text field, type $xTiCl_4in$.

6 In the $x_{0,wHCl}$ text field, type $1e-6$.

Inflow I

1 In the **Model Builder** window, click **Inflow I**.

2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Inflow** section. From the **Mixture specification** list, choose **Mole fractions**.

5 In the x_{0,wN_2} text field, type xN_2in .

6 In the $x_{0,wTiCl_4}$ text field, type $xTiCl_4in$.

7 In the $x_{0,wHCl}$ text field, type $1e-6$.

Outflow I

1 In the **Model Builder** window, click **Outflow I**.

2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Outlet**.

Flux I

1 In the **Model Builder** window, click **Flux I**.

2 In the **Settings** window for **Flux**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Inserts**.

4 Locate the **Mass Transfer to Other Phases** section. Select the **Account for Stefan velocity** checkbox.

5 Locate the **Inward Flux** section. Select the **Species wH₂** checkbox.

6 In the j_{0,wH_2} text field, type $chem.Rwsurf_H2$.

7 Select the **Species wN₂** checkbox.

8 In the j_{0,wN_2} text field, type $chem.Rwsurf_N2$.

9 Select the **Species wTiCl₄** checkbox.

10 In the $j_{0,wTiCl_4}$ text field, type $chem.Rwsurf_TiCl_4$.

11 Select the **Species wHCl** checkbox.

12 In the $j_{0,wHCl}$ text field, type $chem.Rwsurf_HCl$.

Periodic Condition 1

- 1 In the **Model Builder** window, click **Periodic Condition 1**.
- 2 Select Boundaries 1 and 28 only.


SURFACE REACTIONS (SR)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Surface Reactions (sr)**.
- 2 In the **Settings** window for **Surface Reactions**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inserts**.

Surface Properties 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Surface Reactions (sr)** click **Surface Properties 1**.
- 2 In the **Settings** window for **Surface Properties**, click to expand the **Species Conservation on Deforming Geometry** section.
- 3 Locate the **Surface Diffusion** section. In the D_{eTiN} text field, type $1e-7$.

Reactions 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Reactions**.
- 2 In the **Settings** window for **Reactions**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inserts**.
- 4 Locate the **Reaction Rate for Surface Species** section. From the $R_{s,cTiN}$ list, choose **Surface reaction rate for surface species TiN_surf (chem)**.

LAMINAR FLOW (SPF)

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


Inlet 1

In the **Physics** toolbar, click  **Boundaries** and choose **Inlet**.

Outlet 1

In the **Physics** toolbar, click  **Boundaries** and choose **Outlet**.

Periodic Flow Condition 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Flow Condition**.
- 2 In the **Model Builder** window, click **Laminar Flow (spf)**.
- 3 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.
- 4 From the **Compressibility** list, choose **Weakly compressible flow**.
- 5 In the p_{ref} text field, type p_{ref} .

6 In the T_{ref} text field, type Treac.

Fluid Properties 1

- 1 In the **Model Builder** window, click **Fluid Properties 1**.
- 2 In the **Settings** window for **Fluid Properties**, locate the **Fluid Properties** section.
- 3 From the μ list, choose **Dynamic viscosity (chem)**.

Inlet 1

- 1 In the **Model Builder** window, click **Inlet 1**.
- 2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.
- 4 Locate the **Boundary Condition** section. From the list, choose **Mass flow**.
- 5 Clear the **Apply condition on each disjoint selection separately** checkbox.
- 6 Locate the **Mass Flow** section. In the m text field, type mFlowIn.
- 7 Click to expand the **Applicable Pair Region** section. From the **Allowed region** list, choose **All regions**.

Outlet 1

- 1 In the **Model Builder** window, click **Outlet 1**.
- 2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet**.

Periodic Flow Condition 1

- 1 In the **Model Builder** window, click **Periodic Flow Condition 1**.
- 2 Select Boundaries 1 and 28 only.

MESH 1

Size 1

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

Size


- 1 In the **Settings** window for **Size**, locate the **Element Size** section.
- 2 From the **Calibrate for** list, choose **Fluid dynamics**.
- 3 From the **Predefined** list, choose **Coarse**.

Size 1

- 1 In the **Model Builder** window, click **Size 1**.

- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 2, 7–9, 11, 12, and 27 only.
- 5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.
- 6 From the **Predefined** list, choose **Fine**.


Free Triangular 1

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.

Size 1

- 1 Right-click **Free Triangular 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **Fluid dynamics**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type 0.0015.
- 7 Select the **Minimum element size** checkbox. In the associated text field, type 0.5E-3.
- 8 Select the **Maximum element growth rate** checkbox.
- 9 Select the **Curvature factor** checkbox. In the associated text field, type 0.5.
- 10 Select the **Resolution of narrow regions** checkbox. In the associated text field, type 0.8.

Free Triangular 2

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Insert Top Bnds**.

Size 1


- 1 Right-click **Free Triangular 2** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **Fluid dynamics**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type 0.004.

- 7 Select the **Minimum element size** checkbox. In the associated text field, type $2.54E-4$.
- 8 Select the **Maximum element growth rate** checkbox.
- 9 Select the **Curvature factor** checkbox. In the associated text field, type 0.5 .

Size 2

- 1 In the **Model Builder** window, right-click **Free Triangular 2** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Edge**.
- 4 From the **Selection** list, choose **Insert Horizontal Edges**.
- 5 Locate the **Element Size** section. Click the **Custom** button.
- 6 Locate the **Element Size Parameters** section.
- 7 Select the **Maximum element size** checkbox. In the associated text field, type 0.00085 .


Boundary Layers 1

- 1 In the **Mesh** toolbar, click  **Boundary Layers**.
- 2 In the **Settings** window for **Boundary Layers**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Insert Top Bnds**.


Boundary Layer Properties

- 1 In the **Model Builder** window, click **Boundary Layer Properties**.
- 2 In the **Settings** window for **Boundary Layer Properties**, locate the **Edge Selection** section.
- 3 From the **Selection** list, choose **Insert Horizontal Edges**.
- 4 Locate the **Layers** section. In the **Number of layers** text field, type 1 .
- 5 From the **Thickness specification** list, choose **First layer**.
- 6 In the **Thickness** text field, type $3E-4$.

Copy Face 1

- 1 In the **Mesh** toolbar, click  **Copy** and choose **Copy Face**.
- 2 In the **Settings** window for **Copy Face**, locate the **Source Boundaries** section.
- 3 From the **Selection** list, choose **Insert Top Bnds**.
- 4 Locate the **Destination Boundaries** section. From the **Selection** list, choose **Insert Bottom Bnds**.


Mapped /

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Mapped**.
- 2 In the **Settings** window for **Mapped**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inserts Vertical Bnds**.

Distribution /

- 1 Right-click **Mapped I** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Edge Selection** section.
- 3 From the **Selection** list, choose **Insert Vertical Edges**.
- 4 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 9.
- 6 In the **Element ratio** text field, type 2.
- 7 Select the **Symmetric distribution** checkbox.


Swept /

- 1 In the **Mesh** toolbar, click  **Swept**.
- 2 In the **Settings** window for **Swept**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Injector**.


Distribution /

- 1 Right-click **Swept I** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Injector**.
- 4 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 10.
- 6 Select the **Symmetric distribution** checkbox.

Convert /

- 1 In the **Mesh** toolbar, click  **Modify** and choose **Convert**.
- 2 In the **Settings** window for **Convert**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Inserts Vertical Bnds**.

Free Tetrahedral /


- 1 In the **Mesh** toolbar, click  **Free Tetrahedral**.

- 2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Rotating Domain**.

Size 1

- 1 Right-click **Free Tetrahedral 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 **Boundary**.
- 4 From the **Selection** list, choose **Sliding Mesh Destination Bnds**.
- 5 Locate the **Element Size** section. Click the **Custom** button.
- 6 Locate the **Element Size Parameters** section.
- 7 Select the **Maximum element size** checkbox. In the associated text field, type 0.00175.

Copy 1

- 1 In the **Mesh** toolbar, click  **Copy** and choose **Copy**.
- 2 In the **Settings** window for **Copy**, locate the **Source Entities** section.
- 3 From the **Selection** list, choose **Sliding Mesh Destination Bnds**.
- 4 Locate the **Destination Entities** section. From the **Selection** list, choose **Sliding Mesh, Source Bnds**.



Free Triangular 3

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Free Triangular**.
- 2 Select Boundary 1 only.

Size 1

- 1 Right-click **Free Triangular 3** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **Fluid dynamics**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type 0.0013.
- 7 Select the **Minimum element size** checkbox. In the associated text field, type 0.0013/2.
- 8 Select the **Maximum element growth rate** checkbox. In the associated text field, type 1.05.


Copy 2

- 1 In the **Mesh** toolbar, click  **Copy** and choose **Copy**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Copy**, locate the **Destination Entities** section.
- 4 Click to select the  **Activate Selection** toggle button.
- 5 Select Boundary 28 only.


Free Tetrahedral 2

In the **Mesh** toolbar, click  **Free Tetrahedral**.

Boundary Layers 2

- 1 In the **Mesh** toolbar, click  **Boundary Layers**.
- 2 In the **Settings** window for **Boundary Layers**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **All domains**.
- 5 Click to expand the **Corner Settings** section. From the **Handling of sharp edges** list, choose **Trimming**.

Boundary Layer Properties

- 1 In the **Model Builder** window, click **Boundary Layer Properties**.
- 2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.
- 3 Click  **Paste Selection**.
- 4 In the **Paste Selection** dialog, type 2-4, 7-9, 11-14, 19, 20, 26, 27, 31-124, 126-129, 131-202 in the **Selection** text field.
- 5 Click **OK**.
- 6 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.
- 7 In the **Number of layers** text field, type 3.
- 8 In the **Thickness adjustment factor** text field, type 4.
- 9 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.


RESULTS

Mesh 1




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

2 Right-click **Results** > **Datasets** and choose **Mesh**.

Mesh plot

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Mesh plot in the **Label** text field.
- 3 Locate the **Plot Settings** section. Select the **Propagate hiding to lower dimensions** checkbox.

Mesh 1

- 1 Right-click **Mesh plot** and choose **Mesh**.
- 2 In the **Settings** window for **Mesh**, locate the **Level** section.
- 3 From the **Level** list, choose **Volume**.
- 4 Locate the **Coloring and Style** section. From the **Element color** list, choose **Size**.
- 5 From the **Color table** list, choose **TrafficLight**.
- 6 From the **Color table transformation** list, choose **Reverse**.
- 7 Click to expand the **Element Filter** section. Select the **Enable filter** checkbox.
- 8 In the **Expression** text field, type $z < 0$.
- 9 Click the  **Show Grid** button in the **Graphics** toolbar.
- 10 In the **Mesh plot** toolbar, click  **Plot**.
- 11 Click the  **Zoom Extents** button in the **Graphics** toolbar.

STUDY 1 - STATIONARY INSERT SECTIONS


- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type Study 1 - Stationary Insert Sections in the **Label** text field.
- 3 Locate the **Study Settings** section. Select the **Store complete solver history** checkbox.

Solution 1 (sol1)

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

Step 1: Stationary

- 1 In the **Model Builder** window, under **Study 1 - Stationary Insert Sections** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Surface Reactions (sr)**.




- 4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 5 Click  **Add**.
- 6 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|-------------------------|----------------------|----------------|
| mfac (Mass flow factor) | 1/5 1/2 1 2 5 | |



- 7 In the **Study** toolbar, click  **Compute**.

RESULTS



Exterior Walls

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, type Exterior Walls in the **Label** text field.
- 3 Locate the **Selection** section. Click  **Clear Selection**.
- 4 Click  **Paste Selection**.
- 5 In the **Paste Selection** dialog, type 33-44, 49, 50, 55-66, 73-77, 80-82, 85-89, 91-95, 97-106, 110-114, 120-124, 131, 134-137, 139-143, 145, 146, 150-158, 160-167, 174, 177-186, 191, 192, 197-202 in the **Selection** text field.
- 6 Click **OK**.

Exterior Walls I



- 1 Right-click **Exterior Walls** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Selection** section.
- 3 Click  **Clear Selection**.
- 4 Click  **Paste Selection**.
- 5 In the **Paste Selection** dialog, type 2-4, 7-9, 11-14, 19, 20, 26, 27, 31-124, 126-129, 131-202 in the **Selection** text field.
- 6 Click **OK**.

Reactor Walls

- 1 Right-click **Exterior Walls I** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, type Reactor Walls in the **Label** text field.
- 3 Locate the **Selection** section. Click  **Clear Selection**.
- 4 Click  **Paste Selection**.
- 5 In the **Paste Selection** dialog, type 2, 3, 7-9, 11, 13, 14, 19, 26, 31 in the **Selection** text field.

6 Click **OK**.

Study 1, Cut Plane, z = 0

- 1 In the **Results** toolbar, click  **Cut Plane**.
- 2 In the **Settings** window for **Cut Plane**, type Study 1, Cut Plane, z = 0 in the **Label** text field.
- 3 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.
- 4 Click the  **Show More Options** button in the **Model Builder** toolbar.
- 5 In the **Show More Options** dialog, select **Results > Views** in the tree.
- 6 In the tree, select the checkbox for the node **Results > Views**.
- 7 Click **OK**.

View 3D 5

- 1 In the **Model Builder** window, under **Results** right-click **Views** and choose **View 3D**.
- 2 In the **Settings** window for **View 3D**, locate the **View** section.
- 3 Clear the **Show grid** checkbox.

View 3D 6

- 1 Right-click **Views** and choose **View 3D**.
- 2 In the **Settings** window for **View 3D**, locate the **View** section.
- 3 Clear the **Show grid** checkbox.

TiN Deposition Rate

- 1 In the **Model Builder** window, under **Results** click **Concentration, H2, Streamline (tcs)**.
- 2 In the **Settings** window for **3D Plot Group**, type TiN Deposition Rate in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (mfac)** list, choose **1**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Surface and contours: TiN layer growth rate (m/s) Streamline: Velocity field.
- 6 In the **Parameter indicator** text field, type Mass flow factor = eval(mfac).
- 7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 8 Locate the **Color Legend** section. From the **Position** list, choose **Right double**.

Streamline 1

- 1 In the **Model Builder** window, expand the **TiN Deposition Rate** node, then click **Streamline 1**.

- 2 In the **Settings** window for **Streamline**, locate the **Expression** section.
- 3 In the **x-component** text field, type *u*.
- 4 In the **y-component** text field, type *v*.
- 5 In the **z-component** text field, type *w*.
- 6 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.
- 7 In the **Density level** text field, type 8.5.
- 8 From the **Advanced parameters** list, choose **Manual**.
- 9 In the **Terminating distance factor** text field, type 0.25.
- 10 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow length** list, choose **Normalized**.

Color Expression

- 1 In the **Model Builder** window, expand the **Streamline 1** node, then click **Color Expression**.
- 2 In the **Settings** window for **Color Expression**, locate the **Expression** section.
- 3 In the **Expression** text field, type *spf.U*.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Rainbow**.

Selection 1

- 1 In the **Model Builder** window, right-click **Streamline 1** and choose **Selection**.
- 2 Select Domain 4 only.

Surface 1

- 1 In the **Model Builder** window, right-click **TiN Deposition Rate** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type *TiNGrowth*.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Metasepia**.
- 5 From the **Color table transformation** list, choose **Reverse**.
- 6 Click to expand the **Quality** section. From the **Evaluation settings** list, choose **Manual**.
- 7 From the **Smoothing** list, choose **Inside geometry domains**.

Selection 1

- 1 Right-click **Surface 1** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.

- 3 From the **Selection** list, choose **Inserts**.


Surface: Walls

- 1 In the **Model Builder** window, right-click **TiN Deposition Rate** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, type Surface: Walls in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Reactor Walls**.
- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 6 From the **Color** list, choose **Gray**.

Contour 1

- 1 Right-click **TiN Deposition Rate** and choose **Contour**.
- 2 In the **Settings** window for **Contour**, locate the **Expression** section.
- 3 In the **Expression** text field, type TiNgrowth.
- 4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 5 From the **Color** list, choose **Gray**.
- 6 Clear the **Color legend** checkbox.

Selection 1

- 1 Right-click **Contour 1** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Inserts**.
- 4 In the **TiN Deposition Rate** toolbar, click  **Plot**.

Concentration, H2, Surface (tcs), Concentration, HCl, Streamline (tcs), Concentration, HCl, Surface (tcs), Concentration, N2, Streamline (tcs), Concentration, N2, Surface (tcs), Concentration, TiCl4, Streamline (tcs), Concentration, TiCl4, Surface (tcs)

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration, H2, Surface (tcs), Concentration, N2, Streamline (tcs), Concentration, N2, Surface (tcs), Concentration, TiCl4, Streamline (tcs), Concentration, TiCl4, Surface (tcs), Concentration, HCl, Streamline (tcs), and Concentration, HCl, Surface (tcs)**.
- 2 Right-click and choose **Delete**.

Velocity and TiCl4 Mole Fraction

- 1 In the **Settings** window for **3D Plot Group**, type Velocity and TiCl4 Mole Fraction in the **Label** text field.
- 2 Locate the **Data** section. From the **Parameter value (mfac)** list, choose **1**.

- 3 Locate the **Title** section. From the **Title type** list, choose **Manual**.
- 4 In the **Title** text area, type Arrow Surface: Velocity field Slice: Inlet normalized mole fraction of TiCl4.
- 5 In the **Parameter indicator** text field, type Mass flow factor = eval(mfac).
- 6 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 7 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
- 8 Select the **Show units** checkbox.
- 9 Click to expand the **Number Format** section. Select the **Manual color legend settings** checkbox.
- 10 In the **Precision** text field, type 4.

Multislice 1

- 1 In the **Model Builder** window, expand the **Velocity and TiCl4 Mole Fraction** node.
- 2 Right-click **Multislice 1** and choose **Delete**.

Insert Walls

- 1 Right-click **Velocity and TiCl4 Mole Fraction** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, type Insert Walls in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type 1.

Selection 1

- 1 Right-click **Insert Walls** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Inserts**.

Material Appearance 1

- 1 In the **Model Builder** window, right-click **Insert Walls** and choose **Material Appearance**.
- 2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
- 3 From the **Appearance** list, choose **Custom**.
- 4 From the **Material type** list, choose **Gold**.

Reactor Walls

- 1 In the **Model Builder** window, right-click **Velocity and TiCl4 Mole Fraction** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, type Reactor Walls in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Reactor Walls**.

- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 6 From the **Color** list, choose **Gray**.

Velocity, $z = 0$

- 1 Right-click **Velocity and TiCl₄ Mole Fraction** and choose **Arrow Surface**.
- 2 In the **Settings** window for **Arrow Surface**, type *Velocity, $z = 0$* in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 1, Cut Plane, $z = 0$** .
- 4 From the **Solution parameters** list, choose **From parent**.
- 5 Locate the **Expression** section. In the **x-component** text field, type *u*.
- 6 In the **y-component** text field, type *v*.
- 7 In the **z-component** text field, type *w*.
- 8 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 300.
- 9 Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Logarithmic**.
- 10 From the **Color** list, choose **White**.

tcs.x_wTiCl₄/xTiCl₄in

- 1 Right-click **Velocity and TiCl₄ Mole Fraction** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, type *tcs.x_wTiCl₄/xTiCl₄in* in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type *tcs.x_wTiCl₄/xTiCl₄in*.
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.
- 5 In the **Planes** text field, type 1.
- 6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Lagoon**.

Velocity and TiCl₄ Concentration, Periodic Flow

- 1 Right-click **Velocity and TiCl₄ Mole Fraction** and choose **Duplicate**.
- 2 In the **Settings** window for **3D Plot Group**, type *Velocity and TiCl₄ Concentration, Periodic Flow* in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (mfac)** list, choose **5**.
- 4 Locate the **Title** section. In the **Title** text area, type *Slice: Velocity magnitude (m/s) Slice: Mole fraction TiCl₄ Arrow Surface: Velocity field*.
- 5 Locate the **Color Legend** section. Clear the **Show units** checkbox.
- 6 Locate the **Number Format** section. Clear the **Manual color legend settings** checkbox.

Arrow Surface

- 1 In the **Model Builder** window, expand the **Velocity and TiCl₄ Concentration, Periodic Flow** node, then click **Velocity, z = 0**.
- 2 In the **Settings** window for **Arrow Surface**, type Arrow Surface in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **From parent**.
- 4 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 200.
- 5 Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Proportional**.
- 6 From the **Color** list, choose **Gray**.

Selection 1

- 1 Right-click **Arrow Surface** and choose **Selection**.
- 2 Select Boundaries 1 and 28 only.

Slice 1

- 1 In the **Model Builder** window, under **Results > Velocity and TiCl₄ Concentration, Periodic Flow** click **tcs.x_wTiCl₄/xTiCl₄in**.
- 2 In the **Settings** window for **Slice**, type Slice 1 in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type $\text{spf} \cdot U$.
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.
- 5 From the **Entry method** list, choose **Coordinates**.
- 6 In the **y-coordinates** text field, type $\text{range}(0.05, 0.02, 0.11)$.
- 7 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.
- 8 Click to expand the **Quality** section. From the **Evaluation settings** list, choose **Manual**.
- 9 From the **Smoothing** list, choose **Inside geometry domains**.

Selection 1

- 1 Right-click **Slice 1** and choose **Selection**.
- 2 Select Domains 1 and 4 only.

Slice 2

- 1 In the **Model Builder** window, right-click **Velocity and TiCl₄ Concentration, Periodic Flow** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, locate the **Expression** section.
- 3 In the **Expression** text field, type $\text{tcs} \cdot x_w\text{TiCl}_4$.
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.
- 5 In the **Planes** text field, type 1.

- 6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.
- 7 From the **Color table transformation** list, choose **Reverse**.

Partial Pressures

- 1 In the **Model Builder** window, under **Results** click **Pressure (spf)**.
- 2 In the **Settings** window for **3D Plot Group**, type **Partial Pressures** in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (mfac)** list, choose **1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type **Partial Pressure**.
- 6 In the **Parameter indicator** text field, type **Mass flow factor = eval(mfac)**.
- 7 Locate the **Plot Settings** section. From the **View** list, choose **View 3D 5**.
- 8 Clear the **Plot dataset edges** checkbox.
- 9 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
- 10 Select the **Show units** checkbox.
- 11 From the **Position** list, choose **Right double**.
- 12 Locate the **Number Format** section. Select the **Manual color legend settings** checkbox.
- 13 In the **Precision** text field, type **4**.
- 14 Click to expand the **Plot Array** section. From the **Array type** list, choose **Square**.
- 15 From the **Order** list, choose **Column-major**.

----> N2

- 1 Right-click **Partial Pressures** and choose **Annotation**.
- 2 In the **Settings** window for **Annotation**, type ----> N2 in the **Label** text field.
- 3 Locate the **Annotation** section. In the **Text** text field, type **N2**.
- 4 Locate the **Position** section. In the **x** text field, type **-rReactorOut/2**.
- 5 In the **y** text field, type **rReactorOut/2**.
- 6 Click to expand the **Advanced** section. Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 7 From the **Anchor point** list, choose **Center**.
- 8 Right-click ----> N2 and choose **Move Up**.

Insert Walls

- 1 In the **Model Builder** window, under **Results > Partial Pressures** click **Surface**.

- 2 In the **Settings** window for **Surface**, type Insert Walls in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type 1.
- 4 Locate the **Coloring and Style** section. Clear the **Color legend** checkbox.
- 5 Locate the **Quality** section. From the **Smoothing** list, choose **Inside material domains**.
- 6 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Selection 1

- 1 In the **Model Builder** window, expand the **Insert Walls** node, then click **Selection 1**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Inserts**.

Material Appearance 1

- 1 In the **Model Builder** window, right-click **Insert Walls** and choose **Material Appearance**.
- 2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
- 3 From the **Appearance** list, choose **Custom**.
- 4 From the **Material type** list, choose **Gold**.

Reactor Walls

- 1 In the **Model Builder** window, right-click **Partial Pressures** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, type Reactor Walls in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Reactor Walls**.
- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 6 From the **Color** list, choose **Gray**.
- 7 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

pA_N2

- 1 Right-click **Partial Pressures** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, type pA_N2 in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type chem.pA_N2.
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.
- 5 In the **Planes** text field, type 1.
- 6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Metasepia**.
- 7 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

----> TiCl4

- 1 Right-click **Partial Pressures** and choose **Annotation**.
- 2 In the **Settings** window for **Annotation**, type ----> TiCl4 in the **Label** text field.
- 3 Locate the **Annotation** section. In the **Text** text field, type TiCl4.
- 4 Locate the **Position** section. In the **x** text field, type -rReactorOut/2.
- 5 In the **y** text field, type rReactorOut/2.
- 6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 7 From the **Anchor point** list, choose **Center**.
- 8 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.
- 9 In the **Row index** text field, type -1.

Insert Walls 1

- 1 In the **Model Builder** window, right-click **Insert Walls** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 3 In the **Row index** text field, type -1.

Reactor Walls 1

- 1 In the **Model Builder** window, right-click **Reactor Walls** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 3 In the **Row index** text field, type -1.

pA_TiCl4

- 1 In the **Model Builder** window, right-click **pA_N2** and choose **Duplicate**.
- 2 In the **Settings** window for **Slice**, type pA_TiCl4 in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type chem.pA_TiCl4.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Lagoon**.
- 5 Locate the **Plot Array** section. In the **Row index** text field, type -1.

----> H2

- 1 In the **Model Builder** window, right-click ----> TiCl4 and choose **Duplicate**.
- 2 In the **Settings** window for **Annotation**, type ----> H2 in the **Label** text field.
- 3 Locate the **Annotation** section. In the **Text** text field, type H2.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 1.

Insert Walls 2

- 1 In the **Model Builder** window, right-click **Insert Walls 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, type Insert Walls 2 in the **Label** text field.
- 3 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 4 In the **Column index** text field, type 1.

Reactor Walls 2

- 1 In the **Model Builder** window, right-click **Reactor Walls 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, type Reactor Walls 2 in the **Label** text field.
- 3 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 4 In the **Column index** text field, type 1.

pA_H2

- 1 In the **Model Builder** window, right-click **pA_TiCl4** and choose **Duplicate**.
- 2 In the **Settings** window for **Slice**, type pA_H2 in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type chem.pA_H2.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Baptisia**.
- 5 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 6 In the **Column index** text field, type 1.

----> HCl

- 1 In the **Model Builder** window, right-click **----> H2** and choose **Duplicate**.
- 2 In the **Settings** window for **Annotation**, type ----> HCl in the **Label** text field.
- 3 Locate the **Annotation** section. In the **Text** text field, type HCl.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type -1.

Insert Walls 3

- 1 In the **Model Builder** window, right-click **Insert Walls 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, type Insert Walls 3 in the **Label** text field.
- 3 Locate the **Plot Array** section. In the **Row index** text field, type -1.



Reactor Walls 2.1

- 1 In the **Model Builder** window, right-click **Reactor Walls 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 3 In the **Row index** text field, type -1.


pA_HCl

- 1 In the **Model Builder** window, right-click **pA_H2** and choose **Duplicate**.
- 2 In the **Settings** window for **Slice**, type pA_HCl in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type chem.pA_HCl.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type -1.

Partial Pressures

- 1 In the **Model Builder** window, right-click **Partial Pressures** and choose **Move Down**.
- 2 In the **Partial Pressures** toolbar, click  **Plot**.
- 3 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Average Deposition Rates

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type Average Deposition Rates in the **Label** text field.
- 3 Locate the **Transformation** section. From the **Transformation type** list, choose **General**.
- 4 Select the **Keep child nodes** checkbox.

Surface Average 1

- 1 Right-click **Average Deposition Rates** and choose **Average > Surface Average**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 1**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|------------|------|-------------|
| TiNgrowth | um/h | Insert1 |

Surface Average 2

- 1 Right-click **Surface Average 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 2**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|------------|------|-------------|
| TiNgrowth | um/h | Insert2 |

Surface Average 3

- 1 Right-click **Surface Average 2** and choose **Duplicate**.

- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 3**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:


| Expression | Unit | Description |
|------------|------|-------------|
| TiNgrowth | um/h | Insert3 |

Surface Average 4


- 1 Right-click **Surface Average 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 4**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|------------|------|-------------|
| TiNgrowth | um/h | Insert4 |

Average Deposition Rates

- 1 In the **Model Builder** window, click **Average Deposition Rates**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 In the **Expression** text field, type $av1 / av4$.
- 4 In the **Column header** text field, type $Insert1 / Insert4$.
- 5 In the **Average Deposition Rates** toolbar, click  **Evaluate**.

Deposition Variation, Insert 1

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type **Deposition Variation, Insert 1** in the **Label** text field.
- 3 Locate the **Transformation** section. From the **Transformation type** list, choose **General**.
- 4 Select the **Keep child nodes** checkbox.

Surface Maximum 1

- 1 Right-click **Deposition Variation, Insert 1** and choose **Maximum > Surface Maximum**.
- 2 In the **Settings** window for **Surface Maximum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 1**.

4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|------------|------|--------------|
| TiNgrowth | um/h | Maximum rate |

Surface Minimum 1

- 1 In the **Model Builder** window, right-click **Deposition Variation, Insert 1** and choose **Minimum > Surface Minimum**.
- 2 In the **Settings** window for **Surface Minimum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 1**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:


| Expression | Unit | Description |
|------------|------|--------------|
| TiNgrowth | um/h | Minimum rate |

Surface Average 1

- 1 Right-click **Deposition Variation, Insert 1** and choose **Average > Surface Average**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 1**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

| Expression | Unit | Description |
|------------|------|-------------------|
| TiNgrowth | um/h | Average Dep. rate |

Deposition Variation, Insert 1

- 1 In the **Model Builder** window, click **Deposition Variation, Insert 1**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 In the **Expression** text field, type $(\max1 - \min1) / \text{av1}$.
- 4 In the **Column header** text field, type $(\text{Max} - \text{Min}) / \text{Average}$.
- 5 In the **Deposition Variation, Insert 1** toolbar, click  **Evaluate**.

Deposition Variation, Insert 2

- 1 Right-click **Deposition Variation, Insert 1** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Deposition Variation, Insert 1.1**.
- 3 In the **Settings** window for **Evaluation Group**, type **Deposition Variation, Insert 2** in the **Label** text field.

Surface Maximum 1

- 1 In the **Model Builder** window, click **Surface Maximum 1**.
- 2 In the **Settings** window for **Surface Maximum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 2**.


Surface Minimum 1

- 1 In the **Model Builder** window, click **Surface Minimum 1**.
- 2 In the **Settings** window for **Surface Minimum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 2**.

Surface Average 1

- 1 In the **Model Builder** window, click **Surface Average 1**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 2**.

Deposition Variation, Insert 2

- 1 In the **Model Builder** window, click **Deposition Variation, Insert 2**.
- 2 In the **Deposition Variation, Insert 2** toolbar, click  **Evaluate**.

Deposition Variation, Insert 3

- 1 Right-click **Deposition Variation, Insert 2** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Deposition Variation, Insert 2.1**.
- 3 In the **Settings** window for **Evaluation Group**, type **Deposition Variation, Insert 3** in the **Label** text field.

Surface Maximum 1

- 1 In the **Model Builder** window, click **Surface Maximum 1**.
- 2 In the **Settings** window for **Surface Maximum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 3**.

Surface Minimum 1


- 1 In the **Model Builder** window, click **Surface Minimum 1**.
- 2 In the **Settings** window for **Surface Minimum**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Insert 3**.

Surface Average 1

- 1 In the **Model Builder** window, click **Surface Average 1**.
- 2 In the **Settings** window for **Surface Average**, locate the **Selection** section.

3 From the **Selection** list, choose **Insert 3**.

Deposition Variation, Insert 3

- 1** In the **Model Builder** window, click **Deposition Variation, Insert 3**.
- 2** In the **Deposition Variation, Insert 3** toolbar, click  **Evaluate**.

Deposition Variation, Insert 4

- 1** Right-click **Deposition Variation, Insert 3** and choose **Duplicate**.
- 2** In the **Model Builder** window, click **Deposition Variation, Insert 3.1**.
- 3** In the **Settings** window for **Evaluation Group**, type **Deposition Variation, Insert 4** in the **Label** text field.

Surface Maximum 1

- 1** In the **Model Builder** window, click **Surface Maximum 1**.
- 2** In the **Settings** window for **Surface Maximum**, locate the **Selection** section.
- 3** From the **Selection** list, choose **Insert 4**.


Surface Minimum 1

- 1** In the **Model Builder** window, click **Surface Minimum 1**.
- 2** In the **Settings** window for **Surface Minimum**, locate the **Selection** section.
- 3** From the **Selection** list, choose **Insert 4**.


Surface Average 1

- 1** In the **Model Builder** window, click **Surface Average 1**.
- 2** In the **Settings** window for **Surface Average**, locate the **Selection** section.
- 3** From the **Selection** list, choose **Insert 4**.

Deposition Variation, Insert 4

- 1** In the **Model Builder** window, click **Deposition Variation, Insert 4**.
- 2** In the **Deposition Variation, Insert 4** toolbar, click  **Evaluate**.

Average Deposition Rate

- 1** In the **Results** toolbar, click  **ID Plot Group**.
- 2** In the **Settings** window for **ID Plot Group**, type **Average Deposition Rate** in the **Label** text field.
- 3** Locate the **Data** section. From the **Dataset** list, choose **None**.
- 4** Locate the **Plot Settings** section.

- 5 Select the **y-axis label** checkbox. In the associated text field, type **Deposition rate (um/h)**.
- 6 Select the **Two y-axes** checkbox.


Table Graph 1



- 1 Right-click **Average Deposition Rate** and choose **Table Graph**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Source** list, choose **Evaluation group**.
- 4 From the **Plot columns** list, choose **Manual**.
- 5 In the **Columns** list, choose **Insert1 (um/h)**, **Insert2 (um/h)**, **Insert3 (um/h)**, and **Insert4 (um/h)**.
- 6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 7 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
- 8 Click to expand the **Legends** section. Select the **Show legends** checkbox.

Table Graph 2

- 1 In the **Model Builder** window, right-click **Average Deposition Rate** and choose **Table Graph**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Source** list, choose **Evaluation group**.
- 4 From the **Plot columns** list, choose **Manual**.
- 5 In the **Columns** list box, select **Insert1 / Insert4 (1)**.
- 6 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.
- 7 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 8 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
- 9 Locate the **Legends** section. Select the **Show legends** checkbox.

Average Deposition Rate

- 1 In the **Model Builder** window, click **Average Deposition Rate**.
- 2 In the **Average Deposition Rate** toolbar, click  **Plot**.
- 3 In the **Settings** window for **ID Plot Group**, locate the **Axis** section.
- 4 Select the **Manual axis limits** checkbox.
- 5 In the **x minimum** text field, type **0.14277**.
- 6 In the **x maximum** text field, type **5.05723**.
- 7 In the **y minimum** text field, type **0.12960**.

- 8 In the **y maximum** text field, type 0.13998.
- 9 In the **Secondary y minimum** text field, type 0.95.
- 10 In the **Secondary y maximum** text field, type 1.05.
- 11 Locate the **Legend** section. From the **Position** list, choose **Middle right**.
- 12 In the **Average Deposition Rate** toolbar, click  **Plot**.
- 13 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Max-Min Deposition Variation Over Inserts


- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Max-Min Deposition Variation Over Inserts in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Deposition Variation Per Insert.

Table Graph 1

- 1 Right-click **Max-Min Deposition Variation Over Inserts** and choose **Table Graph**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Source** list, choose **Evaluation group**.
- 4 From the **Evaluation group** list, choose **Deposition Variation, Insert 1**.
- 5 From the **Plot columns** list, choose **Manual**.
- 6 In the **Columns** list box, select **(Max-Min)/Average (1)**.
- 7 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 8 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.
- 9 Locate the **Legends** section. Select the **Show legends** checkbox.
- 10 From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:

Legends

Insert 1

Table Graph 2

- 1 Right-click **Table Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Deposition Variation, Insert 2**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends

Insert 2

Table Graph 3

- 1 Right-click **Table Graph 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Deposition Variation, Insert 3**.
- 4 Locate the **Legends** section. In the table, enter the following settings:

Legends

Insert 3

Table Graph 4

- 1 Right-click **Table Graph 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Deposition Variation, Insert 4**.
- 4 Locate the **Legends** section. In the table, enter the following settings:

Legends

Insert 4

- 5 In the **Max-Min Deposition Variation Over Inserts** toolbar, click  **Plot**.

Average Deposition Rate, Max-Min Deposition Variation Over Inserts, Partial Pressures, TiN Deposition Rate, Velocity and TiCl4 Concentration, Periodic Flow, Velocity and TiCl4 Mole Fraction

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **TiN Deposition Rate, Velocity and TiCl4 Mole Fraction, Velocity and TiCl4 Concentration, Periodic Flow, Partial Pressures, Average Deposition Rate, and Max-Min Deposition Variation Over Inserts**.
- 2 Right-click and choose **Group**.

Stationary Insert Sections



In the **Settings** window for **Group**, type Stationary Insert Sections in the **Label** text field.

SURFACE REACTIONS (SR)

Surface Properties 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Surface Reactions (sr)** click **Surface Properties 1**.
- 2 In the **Settings** window for **Surface Properties**, locate the **Species Conservation on Deforming Geometry** section.
- 3 Clear the **Compensate for boundary stretching** checkbox.

ADD STUDY

- 1 In the **Study** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Time Dependent**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Study** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 2 - ROTATING INSERT SECTIONS


- 1 In the **Settings** window for **Study**, type Study 2 - Rotating Insert Sections in the **Label** text field.
- 2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study 2 - Rotating Insert Sections** 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 $0 \text{ } 6 * t_{\text{rot}}$.
- 4 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 5 From the **Method** list, choose **Solution**.
- 6 From the **Study** list, choose **Study 1 - Stationary Insert Sections, Stationary**.
- 7 From the **Solution** list, choose **Solution 1 (sol1)**.
- 8 From the **Parameter value (mfac)** list, choose **1**.


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 **Study 2 - Rotating Insert Sections > Solver Configurations > Solution 2 (sol2)** click **Dependent Variables 1**.
- 4 In the **Settings** window for **Dependent Variables**, locate the **Residual Scaling** section.
- 5 In the **Threshold for updating residual scale** text field, type 1.
- 6 In the **Model Builder** window, under **Study 2 - Rotating Insert Sections > Solver Configurations > Solution 2 (sol2) > Dependent Variables 1** click **Surface Concentration (compl.cTiN)**.
- 7 In the **Settings** window for **Field**, locate the **Scaling** section.
- 8 From the **Method** list, choose **Manual**.
- 9 In the **Scale** text field, type $1e-4$.
- 10 In the **Model Builder** window, under **Study 2 - Rotating Insert Sections > Solver Configurations > Solution 2 (sol2)** click **Time-Dependent Solver 1**.
- 11 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
- 12 From the **Times to store** list, choose **Steps taken by solver**.
- 13 In the **Store every Nth step** text field, type 8.
- 14 Click to expand the **Time Stepping** section. Select the **Initial step** checkbox.
- 15 In the **Study** toolbar, click  **Compute**.

RESULTS

Sector 3D 1


- 1 In the **Results** toolbar, click  **More Datasets** and choose **Sector 3D**.
- 2 In the **Settings** window for **Sector 3D**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 2 - Rotating Insert Sections/Solution 2 (sol2)**.
- 4 Locate the **Symmetry** section. In the **Number of sectors** text field, type 6.
- 5 From the **Sectors to include** list, choose **Manual**.

Study 2/Solution 2, Reactor Walls


- 1 In the **Model Builder** window, under **Results > Datasets** right-click **Study 2 - Rotating Insert Sections/Solution 2 (sol2)** and choose **Duplicate**.
- 2 In the **Settings** window for **Solution**, type Study 2/Solution 2, Reactor Walls in the **Label** text field.

Selection


- 1 In the **Results** toolbar, click  **Attributes** and choose **Selection**.

- 2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Click  **Paste Selection**.
- 5 In the **Paste Selection** dialog, type 2, 3, 7-9, 11-14, 19, 20, 26, 27, 31 in the **Selection** text field.
- 6 Click **OK**.

Sector 3D 2

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Sector 3D**.
- 2 In the **Settings** window for **Sector 3D**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 2/Solution 2, Reactor Walls (sol2)**.
- 4 Locate the **Symmetry** section. In the **Number of sectors** text field, type 6.
- 5 From the **Sectors to include** list, choose **Manual**.

Sector 3D, Cut Plane, $z = 0$

- 1 In the **Results** toolbar, click  **Cut Plane**.
- 2 In the **Settings** window for **Cut Plane**, type Sector 3D, Cut Plane, $z = 0$ in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D I**.
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

Rotating Insert Sections

- 1 In the **Model Builder** window, right-click **Stationary Insert Sections** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Stationary Insert Sections I**.
- 3 In the **Settings** window for **Group**, type Rotating Insert Sections in the **Label** text field.

Full Reactor: Flow and Deposited TiN

- 1 In the **Model Builder** window, under **Results > Rotating Insert Sections** click **TiN Deposition Rate I**.
- 2 In the **Settings** window for **3D Plot Group**, type Full Reactor: Flow and Deposited TiN in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D I**.
- 4 From the **Time (s)** list, choose **Last (90)**.
- 5 Locate the **Title** section. In the **Title** text area, type Velocity, Inlet Normalized TiCl4 Concentration, and Deposited TiN.

- 6 In the **Parameter indicator** text field, type `Time = eval(t) s`.
- 7 Locate the **Plot Settings** section. From the **View** list, choose **View 3D 6**.
- 8 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
- 9 Select the **Show units** checkbox.
- 10 Locate the **Number Format** section. Select the **Manual color legend settings** checkbox.
- 11 In the **Precision** text field, type 4.

Streamline 1

- 1 In the **Model Builder** window, expand the **Full Reactor: Flow and Deposited TiN** node.
- 2 Right-click **Streamline 1** and choose **Delete**.

Insert Walls

- 1 In the **Settings** window for **Surface**, type `Insert Walls` in the **Label** text field.
- 2 Locate the **Expression** section. In the **Expression** text field, type 1.
- 3 Locate the **Quality** section. From the **Smoothing** list, choose **Inside material domains**.

Material Appearance 1

Right-click **Insert Walls** and choose **Material Appearance**.

Material Appearance 1

- 1 In the **Model Builder** window, expand the **Results > Rotating Insert Sections > Full Reactor: Flow and Deposited TiN > Insert Walls** node, then click **Material Appearance 1**.
- 2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
- 3 From the **Appearance** list, choose **Custom**.
- 4 From the **Material type** list, choose **Gold**.

Reactor Walls

- 1 In the **Model Builder** window, under **Results > Rotating Insert Sections > Full Reactor: Flow and Deposited TiN** click **Surface: Walls**.
- 2 In the **Settings** window for **Surface**, type `Reactor Walls` in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D 2**.
- 4 From the **Time (s)** list, choose **0**.

Contour 1



- 1 In the **Model Builder** window, click **Contour 1**.
- 2 In the **Settings** window for **Contour**, locate the **Expression** section.

- 3 In the **Expression** text field, type $c_{TiN} \cdot chem.M_TiN_surf / rho_{TiN}$.
- 4 Locate the **Levels** section. In the **Total levels** text field, type 10.
- 5 Locate the **Coloring and Style** section. From the **Color** list, choose **White**.
- 6 Select the **Color legend** checkbox.

Velocity, $z = 0$

- 1 In the **Model Builder** window, right-click **Full Reactor: Flow and Deposited TiN** and choose **Arrow Surface**.
- 2 In the **Settings** window for **Arrow Surface**, type *Velocity, $z = 0$* in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sector 3D, Cut Plane, $z = 0$** .
- 4 From the **Solution parameters** list, choose **From parent**.
- 5 Locate the **Expression** section. In the **x-component** text field, type u .
- 6 In the **y-component** text field, type v .
- 7 In the **z-component** text field, type w .
- 8 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 400.
- 9 Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Logarithmic**.
- 10 From the **Color** list, choose **White**.

$tcs.x_wTiCl4/xTiCl4in$

- 1 Right-click **Full Reactor: Flow and Deposited TiN** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, type *$tcs.x_wTiCl4/xTiCl4in$* in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type *$tcs.x_wTiCl4/xTiCl4in$* .
- 4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.
- 5 In the **Planes** text field, type 1.
- 6 Locate the **Coloring and Style** section. From the **Color table** list, choose **Lagoon**.
- 7 In the **Full Reactor: Flow and Deposited TiN** toolbar, click  **Plot**.
- 8 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Velocity and TiCl4 Mole Fraction, 90s

- 1 In the **Model Builder** window, under **Results > Rotating Insert Sections** click **Velocity and TiCl4 Mole Fraction I**.
- 2 In the **Settings** window for **3D Plot Group**, type *Velocity and TiCl4 Mole Fraction, 90s* in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Rotating Insert Sections/Solution 2 (sol2)**.
- 4 From the **Time (s)** list, choose **Last (90)**.
- 5 Locate the **Title** section. In the **Parameter indicator** text field, type $\text{Time} = \text{eval}(t) \text{ s}$.

Velocity and TiCl4 Concentration, Periodic Flow 1, Stationary

- 1 In the **Model Builder** window, click **Velocity and TiCl4 Concentration, Periodic Flow 1**.
- 2 In the **Settings** window for **3D Plot Group**, type Velocity and TiCl4 Concentration, Periodic Flow 1, Stationary in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (mfac)** list, choose **1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **Automatic**.


Partial Pressures 1

- 1 In the **Model Builder** window, click **Partial Pressures 1**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 2 - Rotating Insert Sections/Solution 2 (sol2)**.
- 4 From the **Time (s)** list, choose **Last (90)**.
- 5 Locate the **Title** section. In the **Title** text area, type $\text{Time} = \text{eval}(t) \text{ s}$.
- 6 In the **Parameter indicator** text field, type $\text{Time} = \text{eval}(t) \text{ s}$.

Max-Min Deposition Variation Over Inserts 1

In the **Model Builder** window, right-click **Max-Min Deposition Variation Over Inserts 1** and choose **Delete**.

Surface Species Concentration (sr)

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Surface Species Concentration (sr) in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Rotating Insert Sections/Solution 2 (sol2)**.
- 4 From the **Time (s)** list, choose **Last (90)**.
- 5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 6 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
- 7 Select the **Show units** checkbox.
- 8 From the **Position** list, choose **Right double**.

9 Right-click **Surface Species Concentration (sr)** and choose **Move Up**.

Surface I

1 Right-click **Surface Species Concentration (sr)** and choose **Surface**.

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

3 In the **Expression** text field, type **cTiN**.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Metasepia**.

5 From the **Color table transformation** list, choose **Reverse**.

Arrow Volume I

1 In the **Model Builder** window, right-click **Surface Species Concentration (sr)** and choose **Arrow Volume**.

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

3 In the **x-component** text field, type **u**.

4 In the **y-component** text field, type **v**.

5 In the **z-component** text field, type **w**.

6 Locate the **Arrow Positioning** section. Find the **x grid points** subsection. In the **Points** text field, type **5**.

7 Find the **y grid points** subsection. In the **Points** text field, type **8**.

8 Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Logarithmic**.

9 In the **Range quotient** text field, type **500**.

10 From the **Color** list, choose **Custom**.

11 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

12 Click **Define custom colors**.

13 Set the RGB values to **16**, **31**, and **86**, respectively.

14 Click **Add to custom colors**.

15 Click **Show color palette only** or **OK** on the cross-platform desktop.

Slice I

1 Right-click **Surface Species Concentration (sr)** and choose **Slice**.

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

3 In the **Expression** text field, type **spf.U**.

4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

5 In the **Planes** text field, type **1**.

Selection 1

- 1 Right-click **Slice 1** and choose **Selection**.
- 2 Click in the **Graphics** window and then press Ctrl+A to select all domains.

Surface 2

- 1 In the **Model Builder** window, right-click **Surface Species Concentration (sr)** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Reactor Walls**.
- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 6 From the **Color** list, choose **Gray**.

Contour 1

- 1 Right-click **Surface Species Concentration (sr)** and choose **Contour**.
- 2 In the **Settings** window for **Contour**, locate the **Expression** section.
- 3 In the **Expression** text field, type $c_{TiN} \cdot chem.M_{TiN_surf} / \rho_{TiN}$.
- 4 Locate the **Levels** section. In the **Total levels** text field, type 10.
- 5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 6 From the **Color** list, choose **White**.
- 7 Clear the **Color legend** checkbox.

Average Deposition Layer Thickness

- 1 In the **Model Builder** window, right-click **Average Deposition Rates** and choose **Duplicate**.
- 2 In the **Settings** window for **Evaluation Group**, type Average Deposition Layer Thickness in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Rotating Insert Sections/ Solution 2 (sol2)**.
- 4 Locate the **Transformation** section. In the **Expression** text field, type $(av1 - av4) / av1$.
- 5 In the **Column header** text field, type $(av1 - av4) / av1$.

Surface Average 1

- 1 In the **Model Builder** window, expand the **Average Deposition Layer Thickness** node, then click **Surface Average 1**.
- 2 In the **Settings** window for **Surface Average**, locate the **Expressions** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|-------------------------------|------|-------------|
| $cTiN * M_{TiN} / \rho_{TiN}$ | um | Insert1 |

Surface Average 2

- 1 In the **Model Builder** window, click **Surface Average 2**.
- 2 In the **Settings** window for **Surface Average**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

| Expression | Unit | Description |
|-------------------------------|------|-------------|
| $cTiN * M_{TiN} / \rho_{TiN}$ | um | Insert2 |

Surface Average 3

- 1 In the **Model Builder** window, click **Surface Average 3**.
- 2 In the **Settings** window for **Surface Average**, locate the **Expressions** section.
- 3 In the table, enter the following settings:


| Expression | Unit | Description |
|-------------------------------|------|-------------|
| $cTiN * M_{TiN} / \rho_{TiN}$ | um | Insert3 |

Surface Average 4

- 1 In the **Model Builder** window, click **Surface Average 4**.
- 2 In the **Settings** window for **Surface Average**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

| Expression | Unit | Description |
|-------------------------------|------|-------------|
| $cTiN * M_{TiN} / \rho_{TiN}$ | um | Insert4 |

Average Deposition Layer Thickness

- 1 In the **Model Builder** window, click **Average Deposition Layer Thickness**.
- 2 In the **Average Deposition Layer Thickness** toolbar, click  **Evaluate**.

Deposition Layer Thickness



- 1 In the **Model Builder** window, under **Results > Rotating Insert Sections** click **Average Deposition Rate 1**.
- 2 In the **Settings** window for **ID Plot Group**, type Deposition Layer Thickness in the **Label** text field.
- 3 Locate the **Plot Settings** section.

- 4 Select the **y-axis label** checkbox. In the associated text field, type Deposition thickness (um).
- 5 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Table Graph 1

- 1 In the **Model Builder** window, expand the **Deposition Layer Thickness** node, then click **Table Graph 1**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Average Deposition Layer Thickness**.
- 4 In the **Columns** list, choose **Insert1 (um)**, **Insert2 (um)**, **Insert3 (um)**, and **Insert4 (um)**.
- 5 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 6 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

Table Graph 2

- 1 In the **Model Builder** window, click **Table Graph 2**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Average Deposition Layer Thickness**.
- 4 In the **Columns** list box, select **(av1 - av4)/av1 (1)**.
- 5 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 6 Find the **Line markers** subsection. From the **Marker** list, choose **None**.
- 7 In the **Deposition Layer Thickness** toolbar, click  **Plot**.
- 8 Click the  **Zoom Extents** button in the **Graphics** toolbar.