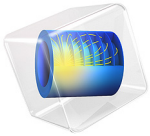

Chemical Vapor Deposition of GaAs

Introduction

This example illustrates the modeling of a reactor for chemical vapor deposition (CVD). CVD is an important process for the electronics industry in which a thin film is grown on a substrate by allowing molecules and molecular fragments to adsorb and react on a surface. Combining detailed chemical reaction kinetics with transport models of a CVD reactor allows for realistic modeling of the deposition process. Such simulations in turn minimize the large number of expensive and time-consuming trial runs typically required for a reactor design.

In the CVD process described here, triethyl-gallium ($Ga(C_2H_5)_3$) first decomposes into a gas phase. The reaction products, along with arsine (AsH_3), then adsorb and react on a substrate to form GaAs layers. The CVD system is modeled using momentum, energy, and mass balances including a detailed description of the gas phase and adsorption kinetics (Ref. 1).

The model highlights the usability of the Reaction Engineering and Chemistry interfaces together with the Reversible Reaction Group feature for simulation of reaction/transport systems in well-mixed (0D) and space-dependent reactors.

In the Reaction Engineering interface you can easily study the transient behavior of different sets of reactions in a perfectly mixed system. The Chemistry interface collects reaction kinetics and calculates transport and thermal parameters, which can seamlessly be coupled with other interfaces. In this application, you also utilize the Reversible Reaction Group feature for CHEMKIN import and organization of the complex system of bulk and surface reactions that are involved in the CVD process. The space-dependent reactor model accounts for mass transport, heat transfer, and fluid flow in the CVD reactor using the Transport of Diluted Species, Heat Transfer in Fluids, and Laminar Flow interfaces.

Model Definition

CHEMISTRY

In this model, the reaction kinetics together with most species transport and thermal properties are imported from CHEMKIN files using the Reversible Reactions Group feature available in either the Reaction Engineering or Chemistry interface. The CHEMKIN reaction kinetics file includes the following reactions making up the CVD process.

1 The gas phase decomposition of $Ga(C_2H_5)_3$:

$$Ga(C_2H_5)_3 \xrightarrow{k_1} Ga(C_2H_5)_2 + C_2H_5^{\bullet} \quad (1)$$

$$Ga(C_2H_5)_2 \xrightarrow{k_2} Ga(C_2H_5)H + C_2H_4 \quad (2)$$

$$Ga(C_2H_5)H \xrightarrow{k_3} GaH_2 + C_2H_4 \quad (3)$$

2 Gas phase radical reactions:

$$C_2H_5^{\bullet} + H_2 \underset{k_4^r}{\overset{k_4^f}{\rightleftharpoons}} C_2H_6 + H^{\bullet} \quad (4)$$

$$C_2H_5^{\bullet} + H^{\bullet} \xrightarrow{k_5} 2CH_3^{\bullet} \quad (5)$$

$$CH_3^{\bullet} + H_2 \xrightarrow{k_6} CH_4 + H^{\bullet} \quad (6)$$

$$2CH_3^{\bullet} \xrightarrow{k_7} C_2H_6 \quad (7)$$

$$C_2H_4 + H^{\bullet} \xrightarrow{k_8} C_2H_5^{\bullet} \quad (8)$$

$$2H^{\bullet} + H_2 \xrightarrow{k_9} 2H_2 \quad (9)$$

3 Growth of GaAs at the surface by the adsorption of gas phase species and the subsequent reaction of the surface-bonded molecular fragments. These surface reactions involve the Ga and As species. S_A and S_G represent surface sites, corresponding to dangling bonds of As or Ga atoms, respectively.

$$Ga(C_2H_5)_3 + S_A \xrightarrow{k_{10}} GaC_2H_5{*} + 2C_2H_5^{\bullet} \quad (10)$$

$$Ga(C_2H_5)H + S_A \underset{k_{11}^r}{\overset{k_{11}^f}{\rightleftharpoons}} Ga(C_2H_5)H{*} \quad (11)$$

$$GaH_2 + S_A \xrightarrow{k_{12}} Ga{*} + 2H^{\bullet} \quad (12)$$

$$Ga(C_2H_5)H{*} \xrightarrow{k_{13}} Ga{*} + C_2H_5^{\bullet} + H^{\bullet} \quad (13)$$

$$AsH_3 + S_G \xrightarrow{k_{14}} As^* + 3H^\bullet \tag{14}$$

4 Surface reactions of carbon and hydrogen fragments:

$$C_2H_5^\bullet + S_A \underset{k_{15}^r}{\overset{k_{15}^f}{\rightleftharpoons}} C_2H_{5A}^* \tag{15}$$

$$C_2H_5^\bullet + S_G \underset{k_{16}^r}{\overset{k_{16}^f}{\rightleftharpoons}} C_2H_{5G}^* \tag{16}$$

$$C_2H_{5A}^* \xrightarrow{k_{17}} H_A^* + C_2H_4 \tag{17}$$

$$C_2H_{5G}^* \xrightarrow{k_{18}} H_G^* + C_2H_4 \tag{18}$$

$$H_A^* \xrightarrow{k_{19}} S_A + H^\bullet \tag{19}$$

$$H_G^* \xrightarrow{k_{20}} S_G + H^\bullet \tag{20}$$

5 Surface reactions leading to GaAs growth:

$$GaC_2H_5^* + As^* \xrightarrow{k_{21}} GaAs + C_2H_5^\bullet + S_A + S_G \tag{21}$$

$$Ga^* + As^* \xrightarrow{k_{22}} GaAs + S_A + S_G \tag{22}$$

The reaction rates (SI unit: mol/(m^3·s)) corresponding to the chemistry just described involve the mass action law

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_j} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}}$$

Here, k_j^f and k_j^r denote the forward and reverse rate constants, respectively. The concentration of species i is denoted c_i (SI unit: mol/m^3). The stoichiometric coefficients are denoted ν_{ij}, and are defined as negative for reactants and positive for products. The temperature dependence of the reaction rates is included through Arrhenius expressions for the rate constants:

$$k = AT^n \exp\left(-\frac{E}{R_g T}\right)$$

In this equation, A denotes the frequency factor, T the temperature (K), n the temperature exponent, E the activation energy (SI unit: J/mol), and R_g the ideal gas constant, 8.314 J/(mol·K). The frequency factor is expressed in the units $(\mathrm{m}^3/\mathrm{mol})^{\alpha-1}/\mathrm{s}$, where α is the order of the reaction.

With the CHEMKIN import, the chemical species automatically adapts the following labels, where _1(ads) indicates adsorbed surface species and _Ga_ indicates adsorption at gallium (Ga) sites instead of the more common arsenic (As) sites Figure 1.

$Ga(C_2H_5)_3$	GaC6H15	C_2H_6	C2H6
$Ga(C_2H_5)_2$	GaC4H10	$C_2H_5^{\bullet}$	C2H5
$Ga(C_2H_5)H$	GaC2H6	C_2H_4	C2H4
GaH_2	GaH2	CH_4	CH4
$Ga(C_2H_5)H^*$	GaC2H6	$CH_3^{\bullet}$	CH3
$GaC_2H_5^*$	GaC2H6	H_2	H2
Ga^*	Ga_Ga_1(ads)	$H^{\bullet}$	H
AsH_3	AsH3_1(ads)	$C_2H_5^*$	C2H5_1(ads), C2H5_Ga_1(ads)
As^*	As_1(ads)	H^*	H_1(ads), H_Ga_1(ads)
$GaAs$	GaAs		

Figure 1: Species labels used in the model.

MODEL ANALYSIS

The analysis follows these steps: First, study of the reaction kinetics in an ideal batch reactor using the Reaction Engineering interface. Afterward, setup of a space-dependent

model with the following interfaces to investigate the effects of momentum, heat, and mass transport within the system:

- Chemistry
- Transport of Diluted Species
- Heat Transfer in Fluids
- Laminar Flow

Figure 2 shows the CVD reactor model geometry. The reactor is 40 cm long and 10 cm high. Located in the center is the substrate, 5 cm across and tilted 10° with respect to the vertical position. Gas enters the reactor at the inlet with a velocity of 0.4 m/s and at a pressure of 4000 Pa.

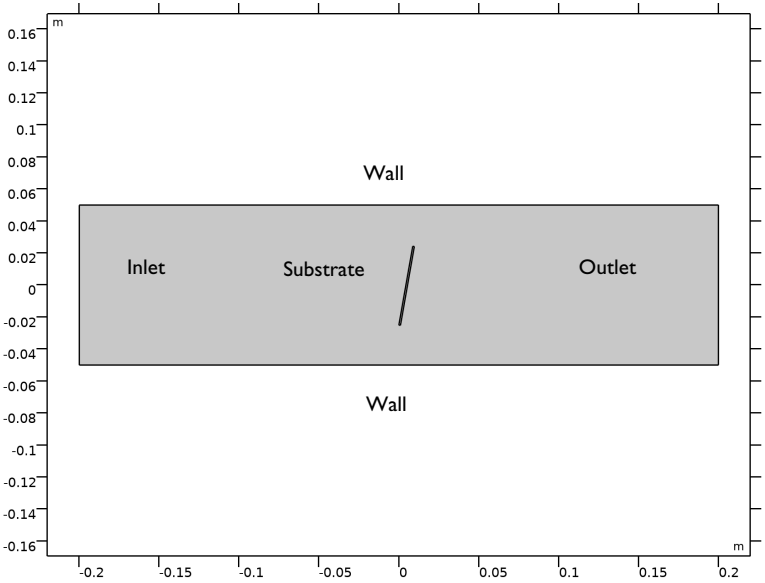

Figure 2: The modeling domain consists of the CVD reactor and the substrate surface.

Results and Discussion

As noted, the first step in the modeling process is to enter the complete set of gas phase reactions, Equation 1 to Equation 9, into the Reaction Engineering interface for analysis. Figure 3 shows the species concentrations as functions of time in a perfectly mixed batch reactor kept at 900 K.

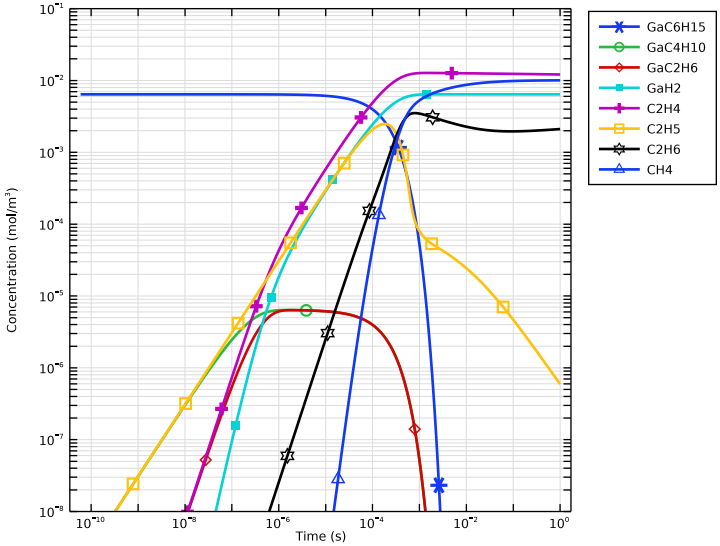

Figure 3: The complete set of gas phase reactions including decomposition reactions of gallium species as well as radical reactions. The chemistry occurs in a perfectly mixed batch reactor held at 900 K. Radical species are not shown in the graph.

As a test, omit the radical reactions given by Equation 4 to Equation 9 from the set of gas phase reactions. Once again analyze the kinetics of the reactions describing gallium species decomposition (Equation 1 to Equation 3) at 900 K. The results appear in Figure 4.

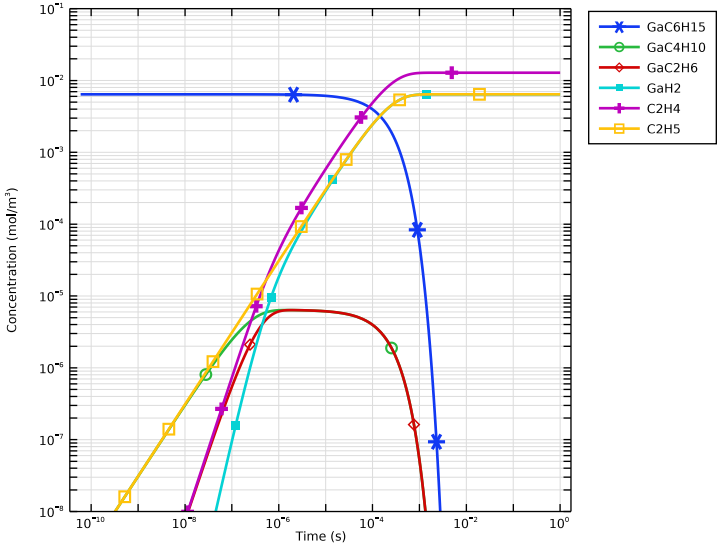

Figure 4: A reduced set of gas phase reactions including only the decomposition reactions of gallium species. Reactions occur in a perfectly mixed system held at 900 K.

Reducing the gas phase reaction set does not affect the reactions of the gallium species. However, excluding the radical reactions has a considerable influence on the carbon-species distribution. For the reduced reaction set, ethene and ethyl radicals are the main carbon products; for the full reaction set the main products are ethene and methane. The various species have different characteristics with respect to surface adsorption and reaction. Furthermore, the net concentration of carbon species is higher for the full reaction set. Both these factors can significantly influence the growth of surface layers. For a first study of geometrical effects on the reacting system, you can bring the reduced reaction model into the actual geometry of the CVD reactor and then solve the space-dependent problem.

The first results from the space-dependent model are displayed below. Figure 5 shows the fluid velocity and Figure 6 the temperature distribution in the reactor domain. The gas mixture enters the reactor with a velocity of 0.4 m/s and a temperature of 300 K with the substrate held at a constant temperature of 900 K. Notice the large effect that the heating plate has on the temperature and the expansion this causes in the fluid. This effect is seen in the average velocity, which increases downstream after the position of the substrate.

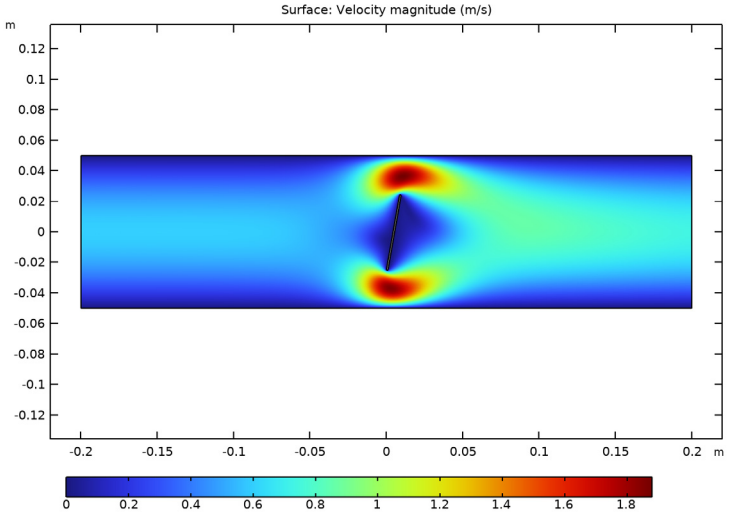

Figure 5: The gas phase velocity in the reactor domain.

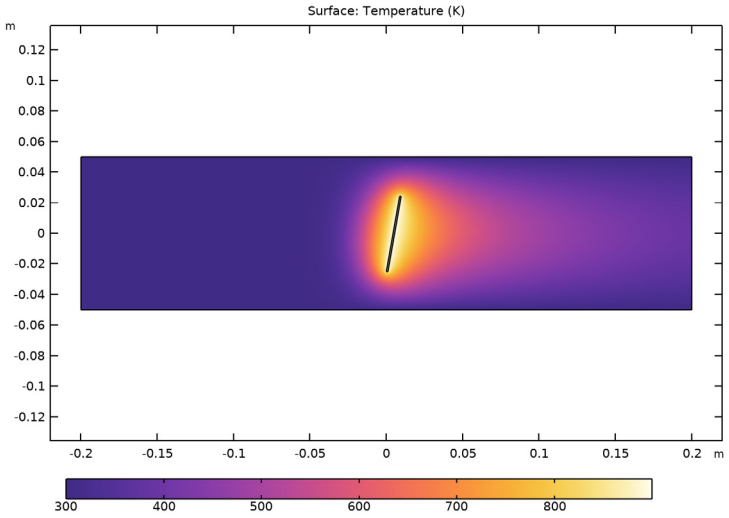

Figure 6: The temperature distribution in the reactor domain.

In Figure 7 shows the concentration distribution of the triethyl-gallium species in the reactor domain, while Figure 8 displays the concentration profile along the reactor

centerline for triethyl-gallium together with that of the final product gallium hydride. Triethyl-gallium is stable at the inlet temperature (300 K) and then rapidly decomposes near the hot substrate.

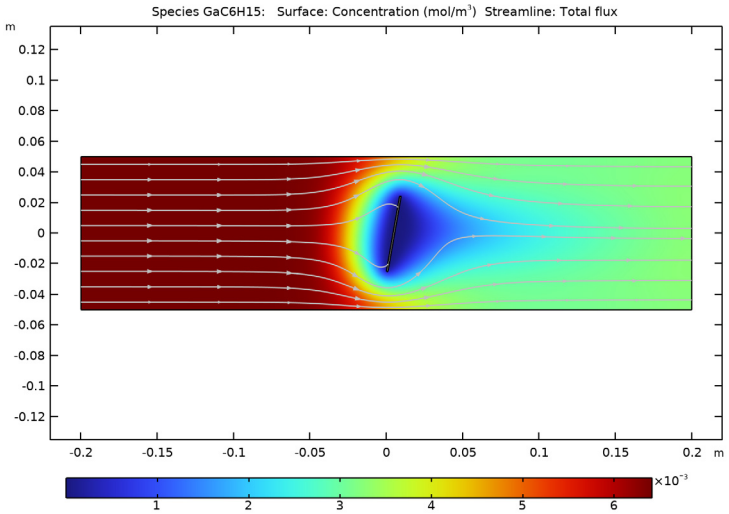

Figure 7: Concentration distribution of triethyl-gallium in the reactor domain.

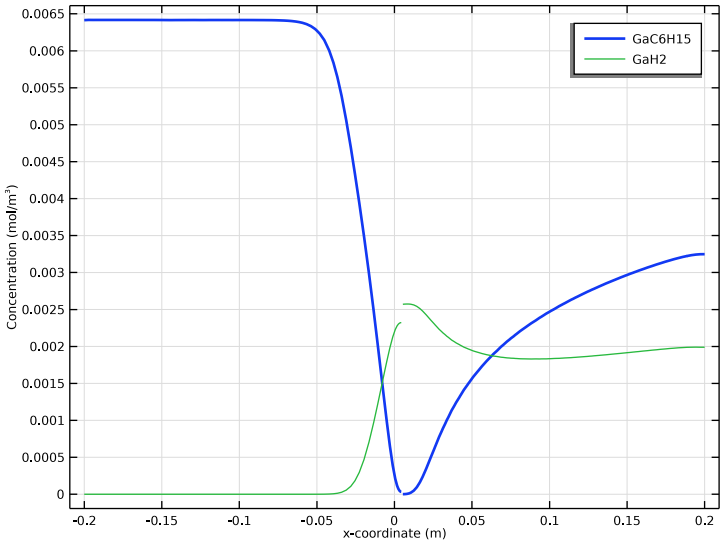

Figure 8: Concentration profiles of triethyl-gallium (blue line) and gallium hydride (green line) along the reactor centerline.

Figure 9 shows the arsine concentration change along the reactor centerline. This species does not decompose in the gas phase. The decrease in concentration at the substrate surface (at the 0 length coordinate) is due to the adsorption of arsine at the surface.

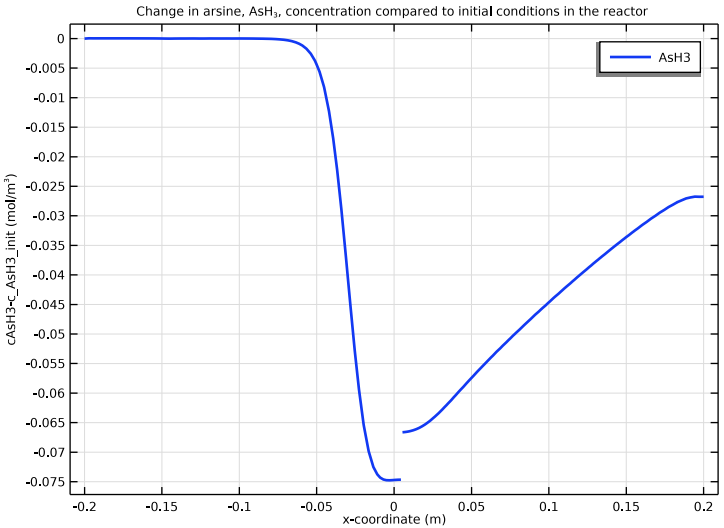

Figure 9: Composition change of arsine along the reactor centerline. Arsine is adsorbed at the substrate surface, which is located at the center of the length scale.

Figure 10 and Figure 11 depict a few of the transport properties calculated in the Chemistry node which are coupled to the physics interfaces of the space-dependent model. Figure 10 shows the diffusivity of triethyl-gallium (bottom) and arsine (top). Figure 11 shows the thermal conductivity of the hydrogen carrier gas. All variables are plotted as functions of temperature.

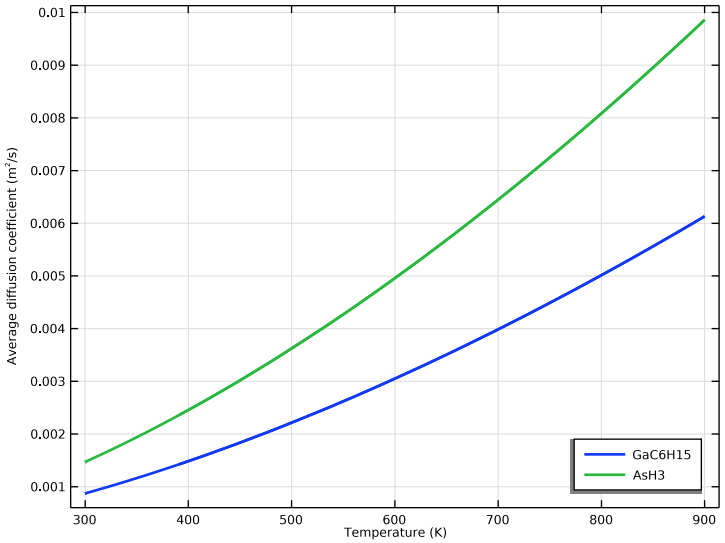

Figure 10: The diffusivities of triethyl-gallium (bottom) and arsine (top) as functions of temperature.

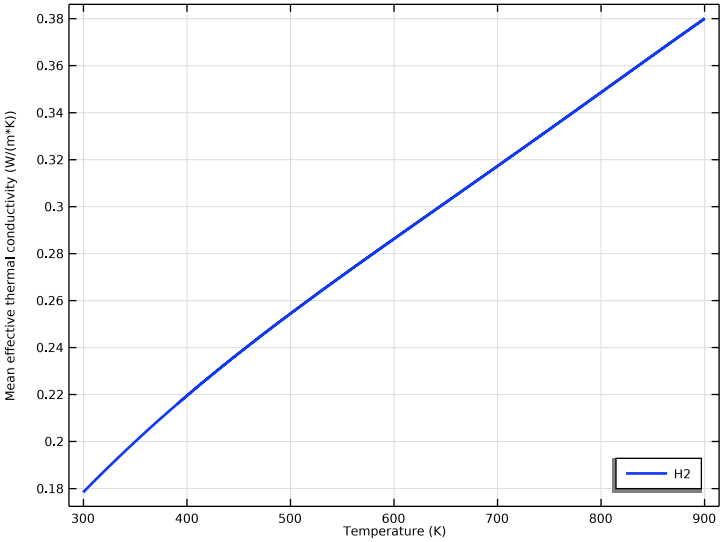

Figure 11: The thermal conductivity of the hydrogen carrier gas.

Reference

1. N.K. Ingle, C. Theodoropoulos, T.J. Mountziaris, R.M. Wexler, and F.T.J. Smith, "Reaction kinetics and transport phenomena underlying the low-pressure metalorganic chemical vapor deposition of GaAs", *J. Crystal Growth*, vol. 167, pp. 543–556, 1996.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/gaas_cvd`

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 **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 Click **Load from File**.

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

The 25 reactions describing the GaAs vapor deposition are available in a kinetics CHEMKIN file. Both bulk and surface reactions are present in this process.

REACTION ENGINEERING - GAS PHASE REACTIONS, FULL SET (RE)

Use the **Reversible Reaction Group** to import the kinetics CHEMKIN file.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, type `Reaction Engineering - Gas Phase Reactions, Full Set (re)` in the **Label** text field.

Reversible Reaction Group 1

1 In the **Reaction Engineering** toolbar, click **Reversible Reaction Group**.

2 In the **Settings** window for **Reversible Reaction Group**, click to expand the **CHEMKIN Import for Kinetics** section.

3 Select the **Import CHEMKIN data** check box.

4 Click **Browse**.

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

6 Click **Import**.

Delete the imported solid species C because it neither takes part in any reactions nor behaviors as third body.

Species: C

In the **Model Builder** window, under **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)** right-click **Species: C** and choose **Delete**.

Species Group 1

First, investigate the bulk reactions at 900 K.

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)>Species Group 1** node, then click **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Energy Balance** section.

3 In the T text field, type `900[K]`.

Remove the imported reactions associated with surface reactions and move reaction 9 to the model builder tree.

Reversible Reaction Group 1

1 In the **Model Builder** window, click **Reversible Reaction Group 1**.

2 In the **Settings** window for **Reversible Reaction Group**, locate the **CHEMKIN Import for Kinetics** section.

3 Clear the **Import CHEMKIN data** check box.

4 Click to expand the **Move Reaction and Species** section. In the **Move reaction (with the number) from table** text field, type `9`.

5 Click **Create Reaction**.

Remove reactions 10 to 25 from the Reaction table by clicking the **Delete** button.

Reaction 9 contains H2 which is the solvent in this process. When moving the reaction from the table a separate feature for the species H2 is created. This can now be accessed and set as solvent.

Species: H2

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

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

3 From the list, choose **Solvent**.

Initial Values 1

Initially, only GaC6H15 and H2 exist in the reactor.

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
GaC6H15	`c_GaC6H15_init`
H2	`c_H2_init`

STUDY (RE)

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

2 In the **Settings** window for **Study**, type `Study (re)` in the **Label** text field.

3 In the **Home** toolbar, click **Compute**.

RESULTS

Gas Phase Concentrations, Full Set (re)

In the **Settings** window for **1D Plot Group**, type `Gas Phase Concentrations, Full Set (re)` in the **Label** text field.

Global 1

Select the species concentrations that are plotted in Figure 3.

1. In the **Model Builder** window, expand the **Gas Phase Concentrations, Full Set (re)** node, then click **Global 1**.
2. In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_GaC6H15 - Concentration - mol/m³**.
3. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_GaC4H10 - Concentration - mol/m³**.
4. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_GaC2H6 - Concentration - mol/m³**.
5. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_GaH2 - Concentration - mol/m³**.
6. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_C2H4 - Concentration - mol/m³**.
7. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_C2H5 - Concentration - mol/m³**.
8. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_C2H6 - Concentration - mol/m³**.
9. Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Full Set (re)>re.c_CH4 - Concentration - mol/m³**.
10. Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.
11. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.
12. From the **Positioning** list, choose **Interpolated**.
13. Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

14 In the table, enter the following settings:

Legends
GaC6H15
GaC4H10
GaC2H6
GaH2
C2H4
C2H5
C2H6
CH4

15 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

16 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

Gas Phase Concentrations, Full Set (re)

1 In the **Model Builder** window, click **Gas Phase Concentrations, Full Set (re)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Axis** section. Select the **Manual axis limits** check box.

5 In the **y minimum** text field, type `1e-8`.

6 In the **y maximum** text field, type `1e-1`.

7 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

8 From the **Position** list, choose **Right**.

9 In the **Gas Phase Concentrations, Full Set (re)** toolbar, click  **Plot**.

To reduce the model before simulating the process in a 2-dimensional model, study whether it is possible to remove the non-gallium species and reactions and yet obtain approximately the same results.

To do so, modify the existing reaction model by first removing reactions of non-gallium species from the **Reversible Reaction Group**. Then solve the mass balances and compare the results with the full reaction model.

REACTION ENGINEERING - GAS PHASE REACTIONS, FULL SET (RE) (RE)

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)** and choose **Copy**.

REACTION ENGINEERING - GAS PHASE REACTIONS, REDUCED SET (RE2)

1 In the **Model Builder** window, right-click **Component 1 (comp1)** and choose **Paste Reaction Engineering**.

2 In the **Messages from Paste** dialog box, click **OK**.

3 In the **Model Builder** window, click **Reaction Engineering - Gas Phase Reactions, Full Set (re) 1 (re2)**.

4 In the **Settings** window for **Reaction Engineering**, type `Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)` in the **Label** text field.

Reversible Reaction Group 1

Remove reactions 4 to 8 from the **Reaction table** by clicking the **Delete** button.

1: 2H+H2=>2H2

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2) (re2)** node.

2 Right-click **1: 2H+H2=>2H2** and choose **Disable**.

ADD STUDY

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

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)**.

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

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

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

STUDY (RE2)

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

2 In the **Settings** window for **Study**, type `Study (re2)` in the **Label** text field.

3 In the **Home** toolbar, click **Compute**.

RESULTS

Gas Phase Concentrations, Reduced Set (re2)

Select the species concentrations that are plotted in Figure 4.

1 In the **Settings** window for **1D Plot Group**, type `Gas Phase Concentrations, Reduced Set (re2)` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Gas Phase Concentrations, Reduced Set (re2)** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_GaC6H15 - Concentration - mol/m³**.

3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_GaC4H10 - Concentration - mol/m³**.

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_GaC2H6 - Concentration - mol/m³**.

5 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_GaH2 - Concentration - mol/m³**.

6 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_C2H4 - Concentration - mol/m³**.

7 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - Gas Phase Reactions, Reduced Set (re2)>re2.c_C2H5 - Concentration - mol/m³**.

8 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

10 From the **Positioning** list, choose **Interpolated**.

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

12 In the table, enter the following settings:

Legends
GaC6H15
GaC4H10
GaC2H6
GaH2

Legends
C2H4
C2H5

13 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

14 Click the  **y-Axis Log Scale** button in the **Graphics** toolbar.

Gas Phase Concentrations, Reduced Set (re2)

1 In the **Model Builder** window, click **Gas Phase Concentrations, Reduced Set (re2)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Axis** section. Select the **Manual axis limits** check box.

5 In the **y minimum** text field, type `1e-8`.

6 In the **y maximum** text field, type `1e-1`.

7 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

8 From the **Position** list, choose **Right**.

9 In the **Gas Phase Concentrations, Reduced Set (re2)** toolbar, click  **Plot**.

A comparison of Figure 3 and Figure 4 reveals that the gallium-related reactions remain approximately the same. This means that you can go on to set up a space-dependent CVD model based on the reduced model instead of the one comprising all bulk species.

Move on to the space-dependent model. This CVD model is in 2D and you set up the necessary reactions using the **Chemistry** interface and the **Reversible Reaction Group** feature. Mass transport, heat transfer, and fluid flow are accounted for with **Transport of Diluted Species**, **Heat Transfer in Fluids**, and **Laminar Flow** interfaces, respectively.

ADD COMPONENT

Right-click **Results>Gas Phase Concentrations, Reduced Set (re2)** and choose **Add Component>2D**.

First, draw the 2D geometry.

GEOMETRY 1

Rectangle 1 (r1)

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

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `0.4`.

4 In the **Height** text field, type `0.1`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 Click **Build Selected**.

Rectangle 2 (r2)

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

2 In the **Settings** window for **Rectangle**, locate the **Position** section.

3 In the **y** text field, type `-0.025`.

4 Locate the **Size and Shape** section. In the **Width** text field, type `1e-3`.

5 In the **Height** text field, type `0.05`.

6 Locate the **Rotation Angle** section. In the **Rotation** text field, type `-10`.

7 Click **Build Selected**.

Difference 1 (dif1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **r1** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Find the **Objects to add** subsection. Click to clear the **Activate Selection** toggle button.

5 Find the **Objects to subtract** subsection. Click to select the **Activate Selection** toggle button.

6 Select the object **r2** only.

Form Union (fin)

In the **Geometry** toolbar, click **Build All**.

Select the **Chemistry** interface and the **Reversible Reaction Group** feature to set up all necessary reaction kinetics and define some species parameters.

ADD PHYSICS

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

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

3 In the tree, select **Chemical Species Transport>Chemistry (chem)**.

4 Click **Add to Component 2** in the window toolbar.

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

Reversible Reaction Group 1

1 Right-click **Component 2 (comp2)>Chemistry (chem)** and choose **Reversible Reaction Group**.

Aside from CHEMKIN import of reaction kinetics, also use CHEMKIN import of transport and thermal properties. In this manner, several thermal and transport properties available in the **Chemistry** interface can be utilized in the other interfaces.

2 In the **Settings** window for **Reversible Reaction Group**, click to expand the **CHEMKIN Import for Kinetics** section.

3 Select the **Import CHEMKIN data** check box.

4 Click **Browse**.

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

6 Click **Import**.

Species: C

1 In the **Model Builder** window, under **Component 2 (comp2)>Chemistry (chem)** right-click **Species: C** and choose **Delete**.

2 In the **Model Builder** window, click **Chemistry (chem)**.

3 In the **Settings** window for **Chemistry**, click to expand the **Calculate Transport Properties** section.

Species Group 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Chemistry (chem)** click **Species Group 1**.

2 In the **Settings** window for **Species Group**, click to expand the **CHEMKIN** section.

3 Click **Browse**.

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

5 Click **Import**.

Species Thermodynamics 1

1 In the **Model Builder** window, expand the **Species Group 1** node, then click **Species Thermodynamics 1**.

2 In the **Settings** window for **Species Thermodynamics**, click to expand the **CHEMKIN Import for Thermodynamic Data** section.

3 Click **Browse**.

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

5 Click **Import**.

Remove the bulk reactions that were considered redundant in the 0D model investigation of the system.

Reversible Reaction Group 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Chemistry (chem)** click **Reversible Reaction Group 1**.

2 In the **Settings** window for **Reversible Reaction Group**, locate the **CHEMKIN Import for Kinetics** section.

3 Clear the **Import CHEMKIN data** check box.

Remove reactions 4 to 8 from the Reaction table by clicking the **Delete** button.

Continue with moving the reactions containing surface species to the model builder tree. This enables access to all surface species. Additionally, do the same with the hydrogen reaction (reaction 17).

4 Click to expand the **Move Reaction and Species** section. In the **Move reaction (with the number) from table** text field, type `9`.

5 Click **Create Reaction**.

Repeat this with reactions 10 to 25.

Disable reaction 17 (`Ga_1(ads)+As_Ga_1(ads)=>GaAs`) and select H2 as solvent.

17: Surface: Ga_1(ads)+As_Ga_1(ads)=>GaAs

In the **Model Builder** window, right-click **17: Surface: Ga_1(ads)+As_Ga_1(ads)=>GaAs** and choose **Disable**.

Species: H2

1 In the **Model Builder** window, right-click **Species: H2** and choose **Enable**.

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

3 From the list, choose **Solvent**.

The surface species concentrations are considered constant. To account for this, lock the concentrations for these.

Species: GaAs

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

2 In the **Settings** window for **Species**, click to expand the **Constant Concentration/Activity** section.

3 Select the **Keep concentration/activity constant** check box.

Repeat the same lock operation for `GaC2H5_1_surf`, `GaC2H6_1_surf`, `Ga_1_surf`, `As_Ga_1_surf`, `C2H5_1_surf`, `C2H5_Ga_1_surf`, `H_1_surf`, and `H_Ga_1_surf`.

4 In the **Model Builder** window, collapse the **Chemistry (chem)** node.

COMPONENT 2 (COMP2)

Add a **Transport of Diluted Species** interface to model the mass transport of the bulk species diluted in solvent. When available, use the transport parameters from the **Chemistry** interface. Additionally, show the **Advanced physics option**. This is needed to choose the conservative form for the convective term in the mass transfer interface. The conservative form should be used for systems including convection and non-negligible changes in density.

ADD PHYSICS

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

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

3 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

4 Click **Add to Component 2** in the window toolbar.

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

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

7 In the **Show More Options** dialog box, select **Physics>Advanced Physics Options** in the tree.

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

9 Click **OK**.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Settings** window for **Transport of Diluted Species**, click to expand the **Advanced Settings** section.

2 From the **Convective term** list, choose **Conservative form**.

3 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type `8`.

4 In the **Concentrations** table, enter the following settings:

cGaC4H10
cC2H5
cH
cC2H4
cAsH3
cGaH2
cGaC2H6
cGaC6H15

Set the constant (locked) concentrations in the **Chemistry** interface main node.

CHEMISTRY (CHEM)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry (chem)**.

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

3 From the **Species solved for** list, choose **Transport of Diluted Species**.

4 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)
AsH3	Variable	cAsH3	Solved for
C2H4	Variable	cC2H4	Solved for
C2H5	Variable	cC2H5	Solved for
GaAs	Constant	User defined	0
GaC2H6	Variable	cGaC2H6	Solved for
GaC4H10	Variable	cGaC4H10	Solved for
GaC6H15	Variable	cGaC6H15	Solved for
GaH2	Variable	cGaH2	Solved for
H	Variable	cH	Solved for
H2	Solvent	User defined	c_H2_init

5 Find the **Surface species** subsection. In the table, enter the following settings:

Species	Species concentration type	Surface concentration (mol/m^2)
As_Ga_1(ads)	Constant	c_Assurf_Ga
C2H5_1(ads)	Constant	c_C2H5surf

Species	Species concentration type	Surface concentration (mol/m^2)
C2H5_Ga_1(ads)	Constant	c_C2H5surf_Ga
GaC2H5_1(ads)	Constant	c_GaC2H5surf
GaC2H6_1(ads)	Constant	0
Ga_1(ads)	Constant	c_Gasurf
H_1(ads)	Constant	c_Hsurf
H_Ga_1(ads)	Constant	c_Hsurf_Ga

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

1 In the **Model Builder** window, under **Component 2 (comp2)> Transport of Diluted Species (tds)** click **Transport Properties 1**.

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

3 From the **Source** list, choose **Chemistry**.

4 From the D_{cGaC4H10} list, choose **Diffusion coefficient , GaC4H10 in H2 (solvent) (chem)**.

5 From the D_{cC2H5} list, choose **Diffusion coefficient , C2H5 in H2 (solvent) (chem)**.

6 From the D_{cH} list, choose **Diffusion coefficient , H in H2 (solvent) (chem)**.

7 From the D_{cC2H4} list, choose **Diffusion coefficient , C2H4 in H2 (solvent) (chem)**.

8 From the D_{cAsH3} list, choose **Diffusion coefficient , AsH3 in H2 (solvent) (chem)**.

9 From the D_{cGaH2} list, choose **Diffusion coefficient , GaH2 in H2 (solvent) (chem)**.

10 From the D_{cGaC2H6} list, choose **Diffusion coefficient , GaC2H6 in H2 (solvent) (chem)**.

11 From the D_{cGaC6H15} list, choose **Diffusion coefficient , GaC6H15 in H2 (solvent) (chem)**.

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Reaction Rates** section. From the R_{cGaC4H10} list, choose **Reaction rate for species GaC4H10 (chem)**.

5 From the R_{cC2H5} list, choose **Reaction rate for species C2H5 (chem)**.

6 From the R_{cH} list, choose **Reaction rate for species H (chem)**.

7 From the R_{cC2H4} list, choose **Reaction rate for species C2H4 (chem)**.

8 From the R_{cAsH3} list, choose **Reaction rate for species AsH3 (chem)**.

9 From the R_{cGaH2} list, choose **Reaction rate for species GaH2 (chem)**.

10 From the R_{cGaC2H6} list, choose **Reaction rate for species GaC2H6 (chem)**.

11 From the R_{cGaC6H15} list, choose **Reaction rate for species GaC6H15 (chem)**.

Surface Reactions 1

Create a **Surface Reactions** feature and apply it at the substrate surface. Then prescribe the surface reaction rates to model the deposition on the substrate.

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

2 Select Boundaries 4–7 only.

3 In the **Settings** window for **Surface Reactions**, locate the **Surface Reaction Rate** section.

4 From the $J_{0,\mathrm{cGaC4H10}}$ list, choose **Surface reaction rate for species GaC4H10 (chem)**.

5 From the $J_{0,\mathrm{cC2H5}}$ list, choose **Surface reaction rate for species C2H5 (chem)**.

6 From the $J_{0,\mathrm{cH}}$ list, choose **Surface reaction rate for species H (chem)**.

7 From the $J_{0,\mathrm{cC2H4}}$ list, choose **Surface reaction rate for species C2H4 (chem)**.

8 From the $J_{0,\mathrm{cAsH3}}$ list, choose **Surface reaction rate for species AsH3 (chem)**.

9 From the $J_{0,\mathrm{cGaH2}}$ list, choose **Surface reaction rate for species GaH2 (chem)**.

10 From the $J_{0,\mathrm{cGaC2H6}}$ list, choose **Surface reaction rate for species GaC2H6 (chem)**.

11 From the $J_{0,\mathrm{cGaC6H15}}$ list, choose **Surface reaction rate for species GaC6H15 (chem)**.

Inflow 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

4 In the $c_{0,\mathrm{cAsH3}}$ text field, type `c_AsH3_in`.

5 In the $c_{0,\mathrm{cGaC6H15}}$ text field, type `c_GaC6H15_in`.

Outflow 1

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

2 Select Boundary 8 only.

Initial Values 1

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

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

3 In the $cAsH3$ text field, type `c_AsH3_in`.

4 In the $cGaC6H15$ text field, type `c_GaC6H15_in`.

COMPONENT 2 (COMP2)

Add a **Heat Transfer in Fluids** interface to model the heat transfer and heat generation in the reactor. When available, use the thermal parameters from the **Chemistry** interface.

ADD PHYSICS

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

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

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

4 Click **Add to Component 2** in the window toolbar.

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

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Heat Transfer in Fluids (ht)** click **Fluid 1**.

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

3 From the k list, choose **Thermal conductivity (chem)**.

4 Locate the **Thermodynamics, Fluid** section. From the **Fluid type** list, choose **Gas/Liquid**.

5 From the ρ list, choose **Density (chem)**.

6 From the C_p list, choose **Heat capacity at constant pressure (chem)**.

7 From the γ list, choose **User defined**.

Heat Source 1

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

2 Select Domain 1 only.

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

4 From the Q_0 list, choose **Heat source of reactions (chem)**.

Temperature 1

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

2 Select Boundaries 1–3 only.

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

4 In the T_0 text field, type `T_in`.

Temperature 2

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

2 Select Boundaries 4–7 only.

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

4 In the T_0 text field, type `T_surf`.

Outflow 1

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

2 Select Boundary 8 only.

Initial Values 1

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

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

3 In the T text field, type `T_in`.

COMPONENT 2 (COMP2)

Add a **Laminar Flow** interface to model the fluid flow. When available, use the fluid parameters from the **Chemistry** interface.

ADD PHYSICS

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

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

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

4 Click **Add to Component 2** in the window toolbar.

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

LAMINAR FLOW (SPF)

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

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

3 In the p_{ref} text field, type `0[atm]`.

Fluid Properties 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Laminar Flow (spf)** click **Fluid Properties 1**.

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

3 From the ρ list, choose **Density (chem)**.

4 From the μ list, choose **Dynamic viscosity (chem)**.

Inlet 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `u_in`.

Outlet 1

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

2 Select Boundary 8 only.

3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

4 In the p_0 text field, type `p_0`.

5 Select the **Normal flow** check box.

Initial Values 1

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

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

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

CHEMISTRY (CHEM)

Finish the space-dependent model setup by coupling the interfaces.

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Model Input** section.

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

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

Set the density dependent on both pressure and temperature.

5 Locate the **Mixture Properties** section. From the **Density** list, choose **User defined**.

6 In the ρ text field, type `chem.p/R_const/chem.T*chem.M_H2`.

MULTIPHYSICS

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain> Nonisothermal Flow**.

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

MESH 1

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Finer**.

4 Click **Build All**.

STUDY (RE)

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study (re)** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Reaction Engineering - Gas Phase Reactions, Reduced Set (re2) (re2)**, **Chemistry (chem)**, **Transport of Diluted Species (tds)**, and **Heat Transfer in Fluids (ht)**.

ROOT

Solve the model for stationary conditions by selecting the **Stationary** study type.

ADD STUDY

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

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Reaction Engineering - Gas Phase Reactions, Full Set (re) (re)** and **Reaction Engineering - Gas Phase Reactions, Reduced Set (re2) (re2)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

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

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

STUDY 2D MODEL

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

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

3 In the **Home** toolbar, click **Compute**.

RESULTS

Velocity (spf)

To create Figure 5, follow these steps:

1. In the **Model Builder** window, under **Results** click **Velocity (spf)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
3. From the **Position** list, choose **Bottom**.
4. In the **Velocity (spf)** toolbar, click **Plot**.
5. Click the **Zoom Extents** button in the **Graphics** toolbar.

Temperature (ht)

To reproduce Figure 6, do the following:

1. In the **Model Builder** window, click **Temperature (ht)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
3. From the **Position** list, choose **Bottom**.
4. In the **Temperature (ht)** toolbar, click **Plot**.
5. Click the **Zoom Extents** button in the **Graphics** toolbar.

Concentration, GaC6H15 (tds)

You can reproduce Figure 7 as follows:

1. In the **Model Builder** window, click **Concentration, GaC6H15 (tds)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Color Legend** section.
3. From the **Position** list, choose **Bottom**.

Streamline 1

1. In the **Model Builder** window, expand the **Concentration, GaC6H15 (tds)** node, then click **Streamline 1**.
2. In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
3. From the **Positioning** list, choose **On selected boundaries**.
4. In the **Number** text field, type 10.
5. Locate the **Selection** section. Click to select the **Activate Selection** toggle button.
6. Select Boundary 1 only.
7. Click the **Zoom Extents** button in the **Graphics** toolbar.
8. In the **Concentration, GaC6H15 (tds)** toolbar, click **Plot**.

The pressure variation in this model is small. For clarity, plot the relative pressure instead of the total pressure.

Contour

1 In the **Model Builder** window, expand the **Results>Pressure (spf)** node, then click **Contour**.

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

3 In the **Expression** text field, type `p-p_0`.

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

To produce the remaining figures, illustrating various results along the reactor centerline, use a **Cut Line 2D** dataset.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

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

3 In row **Point 1**, set **x** to `-0.2`.

4 In row **Point 2**, set **x** to `0.2`.

5 Click **Plot**.

Concentration Profiles GaC6H15 and GaH2

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration Profiles GaC6H15 and GaH2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

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

GaC6H15

1 Right-click **Concentration Profiles GaC6H15 and GaH2** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `GaC6H15` in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)>Transport of Diluted Species>Species cGaC6H15> cGaC6H15 - Concentration - mol/m³**.

4 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Geometry>Coordinate>x - x-coordinate**.

5 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
GaC6H15

GaH2

1 In the **Model Builder** window, right-click **Concentration Profiles GaC6H15 and GaH2** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type GaH2 in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)>Transport of Diluted Species>Species cGaH2> cGaH2 - Concentration - mol/m³**.

4 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Geometry>Coordinate>x - x-coordinate**.

5 Locate the **Legends** section. Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
GaH2

Concentration Profiles GaC6H15 and GaH2

1 In the **Model Builder** window, click **Concentration Profiles GaC6H15 and GaH2**.

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

3 From the **Title type** list, choose **None**.

4 In the **Concentration Profiles GaC6H15 and GaH2** toolbar, click **Plot**.

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

Concentration Profile AsH3 Change

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

2 In the **Settings** window for **1D Plot Group**, type Concentration Profile AsH3 Change in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

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

Line Graph 1

1 Right-click **Concentration Profile AsH3 Change** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)> Transport of Diluted Species>Species cAsH3>cAsH3 - Concentration - mol/m³**.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `cAsH3-c_AsH3_init`.

4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Change in arsine, AsH<sub>3</sub>, concentration compared to initial conditions in the reactor`.

6 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Geometry>Coordinate>x - x-coordinate**.

7 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

8 Locate the **Legends** section. Select the **Show legends** check box.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
AsH3

11 In the **Concentration Profile AsH3 Change** toolbar, click **Plot**.

The **Chemistry** node calculates the diffusivities, the thermal conductivity, and other fluid properties, including their temperature dependence. Next, plot the diffusivities along the reactor centerline for two of the species as functions of the temperature.

Diffusivities vs. Temperature

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

2 In the **Settings** window for **1D Plot Group**, type `Diffusivities vs. Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

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

GaC6H15

1 Right-click **Diffusivities vs. Temperature** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `GaC6H15` in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)>Transport of Diluted Species>Species cGaC6H15> tds.Dav_cGaC6H15 - Average diffusion coefficient - m²/s**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Locate the **Legends** section. Select the **Show legends** check box.

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
GaC6H15

10 In the **Diffusivities vs. Temperature** toolbar, click **Plot**.

AsH3

1 In the **Model Builder** window, right-click **Diffusivities vs. Temperature** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type AsH3 in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)>Transport of Diluted Species>Species cAsH3> tds.Dav_cAsH3 - Average diffusion coefficient - m²/s**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Locate the **Legends** section. Select the **Show legends** check box.

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
AsH3

Diffusivities vs. Temperature

1 In the **Model Builder** window, click **Diffusivities vs. Temperature**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Grid** section. Select the **Manual spacing** check box.

5 In the **x spacing** text field, type `100`.

6 In the **y spacing** text field, type `1e-3`.

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

8 In the **Diffusivities vs. Temperature** toolbar, click **Plot**.

Thermal Conductivity H2

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

2 In the **Settings** window for **1D Plot Group**, type `Thermal Conductivity H2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

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

Line Graph 1

1 Right-click **Thermal Conductivity H2** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 2 (comp2)> Heat Transfer in Fluids>Material properties>ht.kmean - Mean effective thermal conductivity - W/(m·K)**.

3 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

4 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 2 (comp2)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

5 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

6 Locate the **Legends** section. Select the **Show legends** check box.

7 From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
H2

Thermal Conductivity H2

1 In the **Model Builder** window, click **Thermal Conductivity H2**.

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

3 From the **Title type** list, choose **None**.

4 In the **Thermal Conductivity H2** toolbar, click **Plot**.