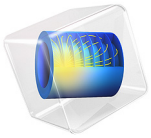

Model created in COMSOL Multiphysics 6.4

Thermal Decomposition of Beta-Carotene in a Flow Reactor

Introduction

This tutorial illustrates how to use the Uncertainty Quantification (UQ) functionality to answer questions regarding sensitivity and reliability of a flow reactor with thermal decomposition. The tutorial investigates which uncertainties in parameters dominate the survival of a nutrient (β-carotene) during a food-processing step. A fluid carrying the nutrient is injected into the reactor, and is subsequently heated by a downstream cylinder. Because β-carotene is heat sensitive it decomposes into fragments, reducing the nutrient level of the fluid. The model starts with a screening study, followed by a sensitivity analysis, then looks at error propagation, and finally performs a reliability analysis.

Model Definition

The system models a plate reactor consisting of a channel in which carrot juice is being heated by a cylinder perpendicular to the juice's direction of flow. The model seeks to answer the question of how much of the nutrient β-carotene is lost due to its thermal decomposition. In this case the outflow rate of remaining β-carotene will be the *Quantity of Interest* (QoI).

The full 3D representation of the reactor geometry is shown in Figure 1.

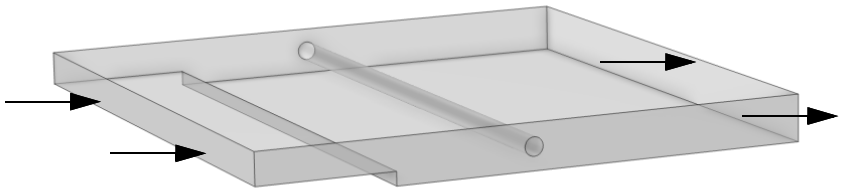

Figure 1: 3D geometry of a parallel plate reactor. The reacting fluid is heated as it passes the cylinder.

CHEMISTRY

A heat-sensitive chemical (β-carotene) undergoes thermal decomposition into fragments (byproduct) according to the following unimolecular reaction in water:

$$\text{betaCarotene} \xRightarrow{k} \text{byproduct}$$

The reaction rate, r, is given by

$$r = kc_{\text{betaCarotene}}$$

where the rate coefficient k is temperature dependent according to the Arrhenius equation:

$$k = A\exp\left(-\frac{E}{R_g T}\right) \tag{1}$$

In Equation 1, A is the frequency factor (9.4×10^{13} 1/s), E the activation energy (110×10^3 J/mol), R_g the gas constant (8.314 J/(mol·K)), and T the temperature (SI unit: K).

In addition, the decomposition reaction is endothermic, and the rate of energy expelled is given by

$$Q = -\text{rate} \cdot H$$

where H is the heat of reaction (8.4 kJ/mol).

The reaction kinetics are set up with the Chemistry interface. The conversion of the species β-carotene in the reactor is a function of the residence time; that is, it depends on the detailed fluid flow. Furthermore, the decomposition is influenced by the temperature distribution.

PARAMETERIZATION

To investigate the performance and reliability of the reactor, a number of parameters in the model setup need to be selected. The uncertainty quantification of the quantity of interest will be evaluated with respect to these inputs. The parameters can, for example, be physical properties of the fluid or the reactor material, such as the fluid viscosity or the heat conductivity of the reactor walls. It can also be parameters defining the reactor configuration, such as the position and radius of the cylinder or the height of the channel. Specific to the field of chemical engineering, parameters used to describe the reaction kinetics, such as reaction rate constants, activation energy, or the enthalpy of reaction, can also be used. Table 1 lists the parameters varied in this model, along with the default values and the respective statistical distributions describing their variation, in this example the distributions are arbitrary and simply used for demonstration purposes. Both the joint

effect and the individual sensitivity of the results on these uncertainties will be studied using the study steps provided by the Uncertainty Quantification Module.

TABLE 1: INPUT PARAMETERS SUBJECT TO UNCERTAINTY QUANTIFICATION

Name	Description	Default value	Distribution
T_cyl	Temperature, heating cylinder	`92[degC]`	Uniform, ±5 K
E	Activation energy	`110[kJ/mol]`	Normal, σ/E=0.3%
A	Frequency factor	`9.4e13[1/s]`	Normal, σ/A=10%
H	Enthalpy of reaction	`8.4[kJ/mol]`	Uniform, ±3%
D_BetaC_ref	Diffusion coefficient	`2.07e-9[m^2/s]`	Normal, σ/ D_BetaC_ref=20%
dDdT	Temperature derivative of diffusion coefficient	`7.5e-11[m^2/s/K]`	Uniform ±50%
xpos	Cylinder x-coordinate	`6[cm]`	Uniform, ±3 cm
ypos	Cylinder y-coordinate	`5[mm]`	Uniform, ±2.25 mm
R1	Cylinder radius	`2[mm]`	Uniform [1 mm, 2.5 mm]

Here, the default values of the Arrhenius parameters are taken from Ref. 1.

THE UNCERTAINTY QUANTIFICATION STUDIES

The Uncertainty Quantification Module provides four different study types:

- Screening, MOAT
  - Identifies the most influential inputs, for each QoI
  - Is based on the Morris One-at-a-Time (MOAT) method
  - Outputs MOAT mean and MOAT standard deviation values for each input investigated
- Sensitivity Analysis
  - Computes the fraction of impact for the inputs, for each QoI
  - Outputs first-order and total Sobol indices
- Uncertainty Propagation
  - Computes the statistical variation of the QoI
  - Outputs a kernel density estimation (KDE) plot representing an estimate of the probability distribution of the QoI

- Reliability Analysis
  - Computes the probability for the fulfillment of a condition based on the QoI
  - For example, what is $P(c < c_{min})$, the probability that the outlet concentration is below some minimum value?

For more information, see the *Uncertainty Quantification Module User's Guide*.

SURROGATE MODELS

To get statistical data based on a physics model, a lot of simulation results are needed where input parameters are varied according to their probability distributions. For a 3D model, this might be computationally infeasible. To get around this problem, the Uncertainty Quantification Module trains a so-called surrogate model, which is used for sensitivity analysis, uncertainty propagation, and reliability analysis (but not for screening).

This process is typically adaptive and the surrogate model can approximate the original model to a user-defined degree of accuracy. The Uncertainty Quantification Module uses two different types of surrogate models:

- Sparse Polynomial Chaos Expansion (SPCE)
  - This surrogate model improves its accuracy by adaptively solving the full model and thereby adding new QoI data using sequential Latin hypercube sampling
- Gaussian Process (GP)
  - This surrogate model improves its accuracy, using information from the current Gaussian Process surrogate model, by adaptively solving the full model for new carefully selected sets of parameter values

Results and Discussion

As a first step, a qualitative screening study is performed. Here the most influential parameters are highlighted, along with the information of what parameters have such a small effect that they can be excluded from further analysis. One of the main benefits of the screening study is that it is computationally cheap. The result of the screening study is a so-called MOAT plot shown in Figure 2. The three parameters with the least impact are

found in the bottom left of the plot. These three parameters (H, D_BetaC_ref, and dDdT) were excluded from further analysis in order to reduce the overall computational cost.

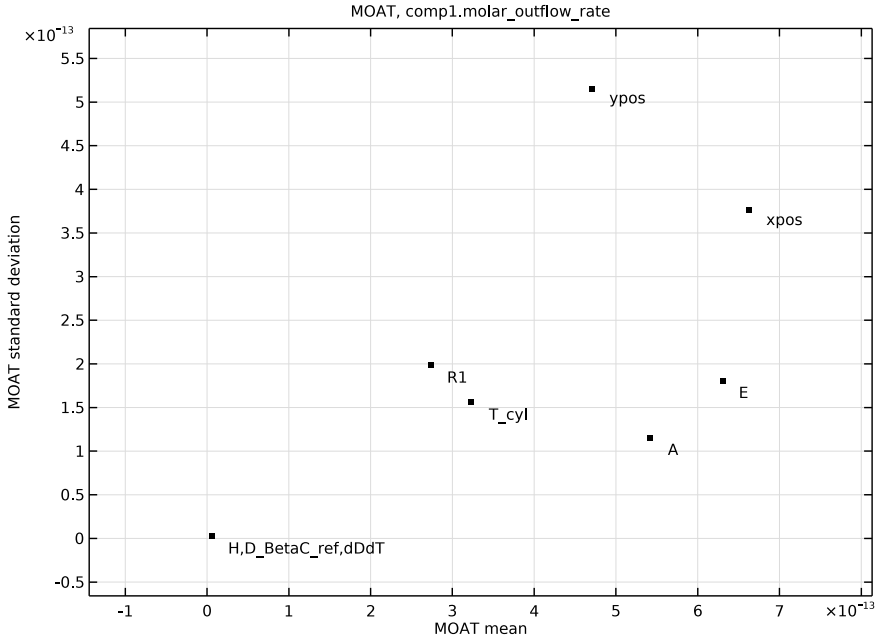

Figure 2: MOAT (Morris one at-a-time) plot from screening study, indicating general effect on x-axis and nonlinearity on y-axis.

After reducing the number of studied parameters, a more rigorous and quantitative Sensitivity Analysis is performed. In this step a surrogate model is trained automatically by COMSOL, and then used internally for a Monte Carlo simulation to perform a great number of evaluations. The output from this study step are the so-called Sobol sensitivity indices which are presented in a bar chart as seen in Figure 3.

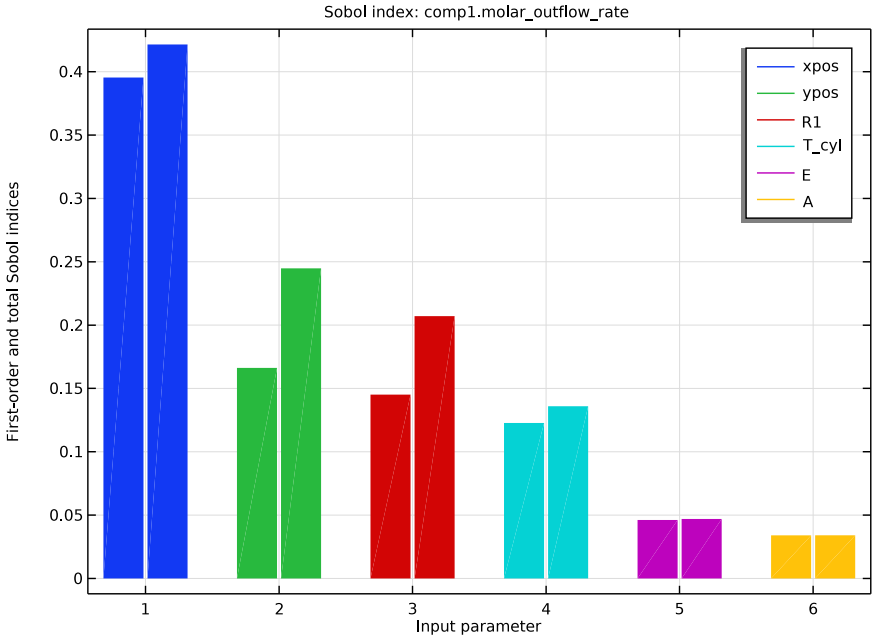

Figure 3: Bar chart of pairs of Sobol indices (first and total order) for each parameter from the sensitivity analysis.

The sum of all first-order Sobol indices (the left bar in each pair) is less than, or equal to, one; only for problems where there are no higher-order interactions between parameters would the value be one. The sum of all total-order Sobol indices (the right bar in each pair) is equal to, or greater than, one. And again, only for additive models would equality hold. The inclusion of higher-order effects in the total index makes differences within pairs useful as an indicator of what parameters interact with the QoI in a nonlinear manner.

The next step is to compute the probability density of the Quantity of Interest. This will provide information about the joint effect of the uncertainties in all varied parameters. Oftentimes, the probability density approximately takes the shape of the normal distribution (bell curve), but skewness and heavy tails are quite common, and it is therefore valuable to study a plot of the distribution. The probability density function is presented in Figure 4.

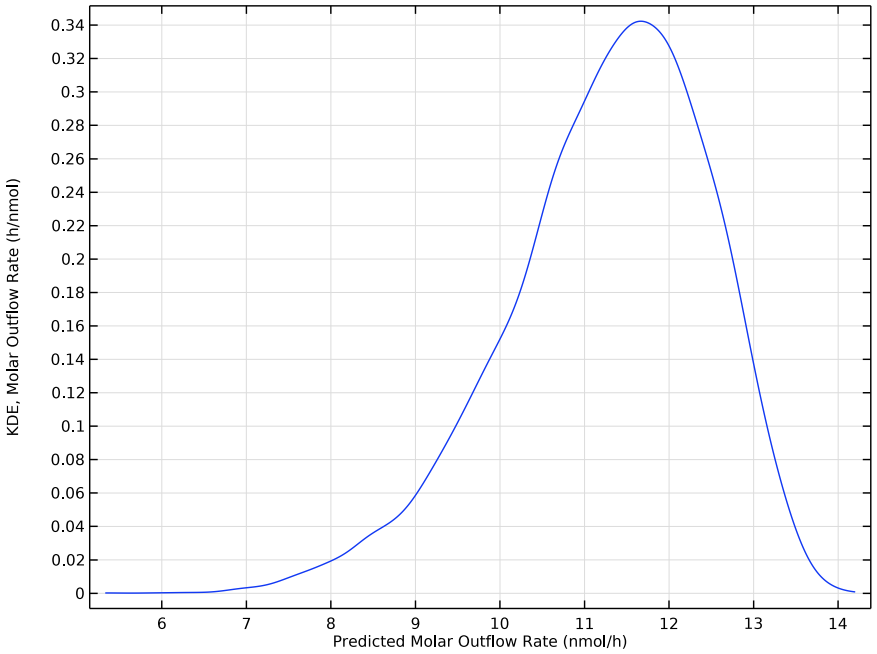

Figure 4: Probability density function, visualizing the distribution of the outflow rate of β-carotene from the reactor (the Quantity of Interest).

Finally a reliability analysis is performed, allowing us to quantify tail risks. In our case, we might want to know how big a risk there is of the β-carotene content dropping below a prescribed threshold. In this model, the risk of the outlet flux dropping below 33% of the inlet was found to be 2%. Note that even though we might be tempted to simply integrate the probability density function up to this threshold, we should refrain from doing so since the tails are not sufficiently sampled in the other study types. The reliability analysis intentionally refines the surrogate model by increasing the sampling in the regions of the multidimensional parameter window yielding these off chance conditions.

It is possible to keep intermediate solutions from the Uncertainty Quantification studies, and it can be quite instructive to compare a set of such results. An example of a plot with multiple such solutions is shown in Figure 5.

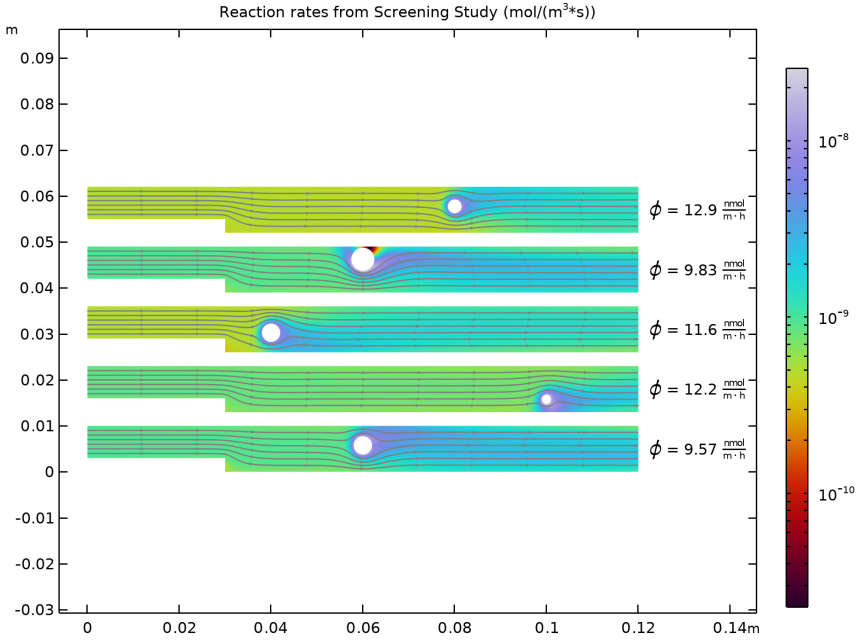

Figure 5: Rate of reaction from a subset of sampled parameters during the screening process.

Reference

1. C. Dhuique-Mayer and others, "Thermal Degradation of Antioxidant Micronutrients in Citrus Juice: Kinetics and Newly Formed Compounds," *J. Agric. Food Chem.*, vol. 55, pp. 4209–4216, 2007.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/thermal_decomposition_uq`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Chemical Species Transport** > **Reacting Flow** > **Laminar Flow, Diluted Species**.

3 Click **Add**.

4 In the **Added physics interfaces** tree, select **Transport of Diluted Species (tds)**.

5 Click **Add Concentration**.

6 In the **Concentrations (mol/m³)** table, enter the following settings:

cBetaC
cByprod

7 In the **Select Physics** tree, select **Heat Transfer** > **Heat Transfer in Fluids (ht)**.

8 Click **Add**.

9 Click **Study**.

10 In the **Select Study** tree, select **General Studies** > **Stationary**.

11 Click **Done**.

GLOBAL DEFINITIONS

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 `thermal_decomposition_uq_parameters.txt`.

GEOMETRY 1

Rectangle 1 (r1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Geometry 1** node.

2 Right-click **Geometry 1** and choose **Rectangle**.

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

4 In the **Width** text field, type `W1`.

5 In the **Height** text field, type `H1`.

Rectangle 2 (r2)

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 `W2`.

4 In the **Height** text field, type `H2`.

Circle 1 (c1)

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

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

3 In the **Radius** text field, type `R1`.

4 Locate the **Position** section. In the **x** text field, type `xpos`.

5 In the **y** text field, type `ypos`.

Line Segment 1 (ls1)

1 In the **Geometry** toolbar, click  **More Primitives** and choose **Line Segment**.

2 On the object **c1**, select Point 3 only.

3 In the **Settings** window for **Line Segment**, locate the **Endpoint** section.

4 From the **Specify** list, choose **Coordinates**.

5 In the **x** text field, type `xpos+10*R1`.

6 In the **y** text field, type `ypos`.

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 Click to select the  **Activate Selection** toggle button for **Objects to subtract**.

5 Select the objects **c1** and **r2** only.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundary 6 only.

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

DEFINITIONS

Inlet

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

2 Right-click **Definitions** and choose **Selections** > **Explicit**.

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

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

5 Select Boundary 1 only.

6 In the **Label** text field, type `Inlet`.

Outlet

1 Right-click **Inlet** and choose **Duplicate**.

2 In the **Settings** window for **Explicit**, type `Outlet` in the **Label** text field.

3 Select Boundary 6 only.

Heater

1 Right-click **Outlet** and choose **Duplicate**.

2 In the **Settings** window for **Explicit**, type `Heater` in the **Label** text field.

3 Select Boundaries 7–9 only.

MESH 1

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

2 Right-click **Component 1 (comp1)** > **Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.

2 Drag and drop **Size 2** below **Size**.

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

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

5 Select Boundary 11 only.

6 Locate the **Element Size** section. From the **Predefined** list, choose **Extra fine**.

7 From the **Calibrate for** list, choose **Fluid dynamics**.

Boundary Layer Properties 1

1 In the **Model Builder** window, expand the **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.

2 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

3 In the **Number of layers** text field, type `3`.

4 In the **Thickness adjustment factor** text field, type `4`.

Boundary Layer Properties 2

1 Right-click **Component 1 (comp1)** > **Mesh 1** > **Boundary Layers 1** > **Boundary Layer Properties 1** and choose **Duplicate**.

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

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

4 Locate the **Layers** section. In the **Number of layers** text field, type `5`.

5 In the **Thickness adjustment factor** text field, type `2`.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, click to expand the **Element Size Parameters** section.

3 In the **Maximum element growth rate** text field, type `1.1`.

4 Click **Build All**.

DEFINITIONS

Variables 1

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`D_BetaC`	`D_BetaC_ref + dDdT*(T-298.15[K])`	m^2/s	`Diffusion coefficient`

ADD MATERIAL

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

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

3 In the **Search** text field, type `water`.

4 Click **Search**.

5 In the tree, select **Built-in** > **Water, liquid**.

6 Click the **Add to Component** button in the window toolbar.

7 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

LAMINAR FLOW (SPF)

Inlet 1

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

2 Select Boundary 1 only.

Outlet 1

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

2 Select Boundary 6 only.

HEAT TRANSFER IN FLUIDS (HT)

Inflow 1

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

2 Select Boundary 1 only.

Outflow 1

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

2 Select Boundary 6 only.

Inflow 1

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

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

3 In the T_{ustr} text field, type `T_inlet`.

Temperature 1

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

2 Select Boundaries 7–9 only.

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

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

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 the **Add to Component 1** button in the window toolbar.

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

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 `betaCarotene=>byproduct`.

4 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.

5 In the A^f text field, type `A`.

6 In the E^f text field, type `E`.

7 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

8 In the H text field, type `H`.

Species: betaCarotene

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

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

3 In the M text field, type `Mn_BetaC`.

Species: byproduct

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

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

3 In the M text field, type `Mn_BetaC`.

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

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

6 Find the **Bulk species** subsection. From the **Species solved for** list, choose **Transport of Diluted Species**.

7 In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)
betaCarotene	Variable	cBetaC	Solved for
byproduct	Variable	cByprod	Solved for

HEAT TRANSFER IN FLUIDS (HT)

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

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 **Material Type** section.

4 From the **Material type** list, choose **Nonsolid**.

5 Locate the **Heat Source** section. From the Q_0 list, choose **Heat of reactions (chem)**.

MULTIPHYSICS

Nonisothermal Flow 1 (nitf1)

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

TRANSPORT OF DILUTED SPECIES (TDS)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport of Diluted Species (tds)** click **Fluid 1**.

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

3 In the D_{cBetaC} text field, type `D_BetaC`.

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 $c_{0,\mathrm{cBetaC}}$ text field, type `cBetaC_inlet`.

Outflow 1

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

2 Select Boundary 6 only.

Reactions 1

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

2 Select Domain 1 only.

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

4 From the R_{cBetaC} list, choose **Reaction rate for species betaCarotene (chem)**.

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

LAMINAR FLOW (SPF)

Inlet 1

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

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

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

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

Outlet 1

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

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

3 Select the **Normal flow** checkbox.

STUDY 1

Step 2: Stationary 1

In the **Model Builder** window, under **Study 1** right-click **Step 1: Stationary** and choose **Duplicate**.

Step 1: Stationary

1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

2 In the **Solve for** column of the table, under **Component 1 (comp1)**, select the checkbox for **Laminar Flow (spf)**.

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Transport of Diluted Species (tds)**, **Heat Transfer in Fluids (ht)**, and **Chemistry (chem)**.

4 In the **Study** toolbar, click **Compute**.

DEFINITIONS

Integration over Exit

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

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

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

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

5 In the **Label** text field, type `Integration over Exit`.

6 In the **Operator name** text field, type `intop_exit`.

Variables 1

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

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`molar_outflow_rate`	`intop_exit(cBetaC*u)`	mol/(m·s)	β-carotene outflow

STUDY 1

In the **Model Builder** window, right-click **Study 1** and choose **More Study Extensions** > **Add Uncertainty Quantification Study Using Study Reference**.

STUDY 2: UQ SCREENING

In the **Settings** window for **Study**, type `Study 2: UQ Screening` in the **Label** text field.

Uncertainty Quantification

1 In the **Model Builder** window, under **Study 2: UQ Screening** click **Uncertainty Quantification**.

2 In the **Settings** window for **Uncertainty Quantification**, locate the **Quantities of Interest** section.

3 Click + **Add**.

4 In the table, enter the following settings:

Expression	Include study-dependent input
`comp1.molar_outflow_rate`	Reduce to single global output

5 Locate the **Input Parameters** section. Click + **Add** nine times.

6 In the table, click to select the cell at row number 1 and column number 3.

7 In the **Lower bound** text field, type `T_cyl-5[K]`.

8 In the **Upper bound** text field, type `T_cyl+5[K]`.

9 In the table, click to select the cell at row number 2 and column number 3.

10 From the **Distribution** list, choose **Normal(μ,σ)**.

11 In the **Mean** text field, type `E`.

12 In the **Standard deviation** text field, type `0.003*E`.

13 In the table, click to select the cell at row number 3 and column number 3.

14 From the **Distribution** list, choose **Normal(μ,σ)**.

15 In the **Mean** text field, type `A`.

16 In the **Standard deviation** text field, type `0.1*A`.

17 In the table, click to select the cell at row number 4 and column number 3.

18 In the **Lower bound** text field, type `0.97*H`.

19 In the **Upper bound** text field, type `1.03*H`.

20 In the table, click to select the cell at row number 5 and column number 3.

21 From the **Distribution** list, choose **Normal(μ,σ)**.

22 In the **Mean** text field, type `D_BetaC_ref`.

23 In the **Standard deviation** text field, type `0.2*D_BetaC_ref`.

24 In the table, click to select the cell at row number 6 and column number 3.

25 In the **Lower bound** text field, type `0.5*dDdT`.

26 In the **Upper bound** text field, type `1.5*dDdT`.

27 In the table, click to select the cell at row number 7 and column number 3.

28 In the **Lower bound** text field, type `4[cm]`.

29 In the **Upper bound** text field, type `10[cm]`.

30 In the table, click to select the cell at row number 8 and column number 3.

31 In the **Lower bound** text field, type `2.75[mm]`.

32 In the **Upper bound** text field, type `7.25[mm]`.

33 In the table, click to select the cell at row number 9 and column number 3.

34 In the **Lower bound** text field, type `1[mm]`.

35 In the **Upper bound** text field, type `2.5[mm]`.

36 Locate the **Output While Solving** section. Select the **Plot** checkbox.

37 In the table, enter the following settings:

Plot group	Plot window
Concentration, BetaC (tds)	Graphics

38 Locate the **Advanced Settings** section. From the **Error handling** list, choose **Skip problematic parameters**.

39 From the **Keep model evaluations in memory** list, choose **All**.

40 In the **Study** toolbar, click **Compute**.

This will produce Figure 2.

STUDY 2: UQ SCREENING

Uncertainty Quantification

1 In the **Model Builder** window, expand the **Results** > **Uncertainty Quantification Graph** > **MOAT, comp1.molar_outflow_rate** node.

2 Right-click **Study 2: UQ Screening** > **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Sensitivity Analysis**.

STUDY 3: UQ SENSITIVITY ANALYSIS

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

2 In the **Settings** window for **Study**, type `Study 3: UQ Sensitivity Analysis` in the **Label** text field.

1 In the **Model Builder** window, under **Study 3: UQ Sensitivity Analysis** click **Uncertainty Quantification**.

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

3 In the table, click to select the cell at row number 4 and column number 3.

4 Click **Delete** three times.

5 In the **Study** toolbar, click **Compute**.

This will produce Figure 3.

STUDY 3: UQ SENSITIVITY ANALYSIS

Uncertainty Quantification

Right-click **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Uncertainty Propagation**.

STUDY 4: UQ UNCERTAINTY PROPAGATION

1 In the **Model Builder** window, click **Study 4: Uncertainty Propagation**.

2 In the **Settings** window for **Study**, type `Study 4: UQ Uncertainty Propagation` in the **Label** text field.

Uncertainty Quantification 3

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

RESULTS

Line Graph 1

1. In the **Model Builder** window, expand the **Results** > **Uncertainty Quantification Graph 2** > **Kernel Density Estimation, QoI1** node, then click **Line Graph 1**.
2. In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3. In the **Expression** text field, type `Kde/1e9/3600`.
4. In the **Description** text field, type `KDE, Molar Outflow Rate (h/nmol)`.
5. Locate the **x-Axis Data** section. In the **Expression** text field, type `predicted*1e9*3600`.
6. In the **Description** text field, type `Predicted Molar Outflow Rate (nmol/h)`.

Kernel Density Estimation, QoI1

1. In the **Model Builder** window, click **Kernel Density Estimation, QoI1**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3. From the **Title type** list, choose **None**.
4. In the **Kernel Density Estimation, QoI1** toolbar, click **Plot**.

   This will produce Figure 4.

STUDY 4: UQ UNCERTAINTY PROPAGATION

Uncertainty Quantification

In the **Model Builder** window, under **Study 4: UQ Uncertainty Propagation** right-click **Uncertainty Quantification** and choose **Add New Uncertainty Quantification Study For** > **Reliability Analysis**.

STUDY 5: UQ RELIABILITY ANALYSIS

1. In the **Model Builder** window, under **Study 5: Reliability Analysis, EGRA** click **Uncertainty Quantification**.
2. In the **Settings** window for **Uncertainty Quantification**, locate the **Quantities of Interest** section.
3. In the table, enter the following settings:

Function name	Expression	Include study-dependent input	True if	Threshold
	`comp1.molar_outflow_rate`	Reduce to single global output	Smaller than threshold	`8[nmol/h]`

4. In the **Model Builder** window, click **Study 5: Reliability Analysis, EGRA**.

5 In the **Settings** window for **Study**, type `Study 5: UQ Reliability Analysis` in the **Label** text field.

Uncertainty Quantification 4

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

RESULTS

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

Reaction Rate

1 In the **Model Builder** window, expand the **Results** > **Tables** > **Reliability Analysis** node.

2 Right-click **Results** and choose **2D Plot Group**.

3 In the **Settings** window for **2D Plot Group**, type `Reaction Rate` in the **Label** text field.

4 Locate the **Data** section. From the **Dataset** list, choose **None**.

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

6 In the **Title** text area, type `Reaction rates from Screening Study (mol/(m<sup>3</sup>*s))`.

7 Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.

8 From the **Array axis** list, choose **y**.

Surface 1

1 Right-click **Reaction Rate** and choose **Surface**.

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

3 From the **Dataset** list, choose **Study 2: UQ Screening/Parametric Solutions 1 (sol4)**.

4 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **1: T_cyl=360.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8652 J/mol, D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00575 m, R1=0.002 m**.

5 Locate the **Expression** section. In the **Expression** text field, type `-tds.R_cBetaC`.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **PrismDark**.

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

8 From the **Scale** list, choose **Logarithmic**.

9 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Surface 2

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

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **10: T_cyl=366.82 K, E=1.1014E5 J/mol, A=1.2305E14 1/s, H=8316 J/mol, D_BetaC_ref=2.2479E-9 m^2/s, dDdT=8.75E-11 m^2/(s*K), xpos=0.1 m, ypos=0.00275 m, R1=0.001 m**.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

5 Locate the **Plot Array** section. In the **Index** text field, type 1.

Surface 3

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

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **20: T_cyl=360.15 K, E=1.1102E5 J/mol, A=9.804E13 1/s, H=8652 J/mol, D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.04 m, ypos=0.00425 m, R1=0.002 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 2.

Surface 4

1 Right-click **Surface 3** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **30: T_cyl=370.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8484 J/mol, D_BetaC_ref=3.3494E-9 m^2/s, dDdT=6.25E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00725 m, R1=0.0025 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 3.

Surface 5

1 Right-click **Surface 4** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **40: T_cyl=363.48 K, E=1.0986E5 J/mol, A=6.4952E13 1/s, H=8148 J/mol, D_BetaC_ref=1.8921E-9 m^2/s, dDdT=1.125E-10 m^2/(s*K), xpos=0.08 m, ypos=0.00575 m, R1=0.0015 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 4.

Streamline 1

1 In the **Model Builder** window, right-click **Reaction Rate** and choose **Streamline**.

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

3 From the **Dataset** list, choose **Study 2: UQ Screening/Parametric Solutions 1 (sol4)**.

4 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **1: T_cyl=360.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8652 J/mol, D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00575 m, R1=0.002 m**.

5 Locate the **Streamline Positioning** section. From the **Entry method** list, choose **Coordinates**.

6 In the **x** text field, type `0 0 0 0 0 0`.

7 In the **y** text field, type `0.004 0.005 0.006 0.007 0.008 0.009`.

8 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **Custom**.

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

10 Click **Define custom colors**.

11 Set the RGB values to 128, 128, and 128, respectively.

12 Click **Add to custom colors**.

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

14 From the **Type** list, choose **Arrow**.

15 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Streamline 2

1 Right-click **Streamline 1** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **10: T_cyl=366.82 K, E=1.1014E5 J/mol, A=1.2305E14 1/s, H=8316 J/mol, D_BetaC_ref=2.2479E-9 m^2/s, dDdT=8.75E-11 m^2/(s*K), xpos=0.1 m, ypos=0.00275 m, R1=0.001 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Streamline 3

1 Right-click **Streamline 2** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **20: T_cyl=360.15 K, E=1.1102E5 J/mol, A=9.804E13 1/s, H=8652 J/mol,**

D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.04 m, ypos=0.00425 m, R1=0.002 m.

4 Locate the **Plot Array** section. In the **Index** text field, type 2.

Streamline 4

1 Right-click **Streamline 3** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **30: T_cyl=370.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8484 J/mol, D_BetaC_ref=3.3494E-9 m^2/s, dDdT=6.25E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00725 m, R1=0.0025 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 3.

Streamline 5

1 Right-click **Streamline 4** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **40: T_cyl=363.48 K, E=1.0986E5 J/mol, A=6.4952E13 1/s, H=8148 J/mol, D_BetaC_ref=1.8921E-9 m^2/s, dDdT=1.125E-10 m^2/(s*K), xpos=0.08 m, ypos=0.00575 m, R1=0.0015 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 4.

Annotation 1

1 In the **Model Builder** window, right-click **Reaction Rate** and choose **Annotation**.

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

3 From the **Dataset** list, choose **Study 2: UQ Screening/Parametric Solutions 1 (sol4)**.

4 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **1: T_cyl=360.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8652 J/mol, D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00575 m, R1=0.002 m**.

5 Locate the **Annotation** section. In the **Text** text field, type `$\phi$ = eval(comp1.molar_outflow_rate, nmol/m/h) $\mathrm{\frac{nmol}{m\cdot h}}$`.

6 Select the **LaTeX markup** checkbox.

7 Locate the **Position** section. In the **x** text field, type `W1`.

8 In the **y** text field, type `H1/2`.

9 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

10 From the **Anchor point** list, choose **Middle left**.

11 Click to expand the **Advanced** section. In the **Precision** text field, type 3.

12 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Annotation 2

1 Right-click **Annotation 1** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **10: T_cyl=366.82 K, E=1.1014E5 J/mol, A=1.2305E14 1/s, H=8316 J/mol, D_BetaC_ref=2.2479E-9 m^2/s, dDdT=8.75E-11 m^2/(s*K), xpos=0.1 m, ypos=0.00275 m, R1=0.001 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 1.

Annotation 3

1 Right-click **Annotation 2** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **20: T_cyl=360.15 K, E=1.1102E5 J/mol, A=9.804E13 1/s, H=8652 J/mol, D_BetaC_ref=7.9064E-10 m^2/s, dDdT=3.75E-11 m^2/(s*K), xpos=0.04 m, ypos=0.00425 m, R1=0.002 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 2.

Annotation 4

1 Right-click **Annotation 3** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **30: T_cyl=370.15 K, E=1.0898E5 J/mol, A=8.996E13 1/s, H=8484 J/mol, D_BetaC_ref=3.3494E-9 m^2/s, dDdT=6.25E-11 m^2/(s*K), xpos=0.06 m, ypos=0.00725 m, R1=0.0025 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type 3.

Annotation 5

1 Right-click **Annotation 4** and choose **Duplicate**.

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

3 From the **Parameter value (T_cyl (K),E (J/mol),A (1/s),H (J/mol),...)** list, choose **40: T_cyl=363.48 K, E=1.0986E5 J/mol, A=6.4952E13 1/s, H=8148 J/mol,**

D_BetaC_ref=1.8921E-9 m^2/s, dDdT=1.125E-10 m^2/(s*K), xpos=0.08 m, ypos=0.00575 m, R1=0.0015 m.

4 Locate the **Plot Array** section. In the **Index** text field, type 4.

Reaction Rate

This is Figure 5.