

Thermophoresis

This model is licensed under the COMSOL Software License Agreement 6.1. All trademarks are the property of their respective owners. See www.comsol.com/trademarks.

Introduction

In a gas at nonuniform temperature, suspended particles tend to move from regions of high temperature to low, due to the *thermophoretic force*. This effect can be used to create thermal precipitators that filter out undesirable particles from a feed gas. It can also be used in chemical vapor deposition, to inhibit the arrival of particle contaminants on the surface of a susceptor. This tutorial predicts the size of a particle-free zone above a heated susceptor for different temperature gradients. The results agree well with Ref. 1.

Note: This application requires the Particle Tracing Module, the Heat Transfer Module, and one of the following: CFD Module, Microfluidics Module, or Plasma Module.

Model Definition

Hydrogen gas is injected into the modeling domain at a flow rate of 2000 scem. The gas flows over a heated susceptor and out through a pump after a 90-degree bend, see Figure 1. Particles are injected into the gas stream at the beginning of the susceptor uniformly in the y direction. The initial particle velocity is set to the fluid velocity.

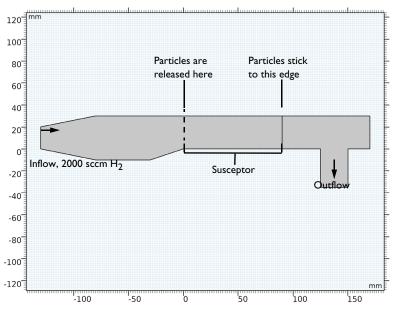


Figure 1: Diagram showing the model geometry (in mm) and location of the susceptor.

DRAG FORCE

The particle positions are computed by solving second-order equations of motion for the particle position vector components, following Newton's second law,

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{v}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}(m_{\mathrm{p}}\mathbf{v}) = \mathbf{F}_{\mathrm{t}}$$

where

- **q** is the particle position (SI unit: m),
- **v** is the particle velocity (SI unit: m/s),
- $m_{\rm p}$ is the particle mass (SI unit: kg), and
- **F**_t is the total force (SI unit: N).

In this example, the total force includes the drag, gravity, and thermophoretic forces,

$$\mathbf{F}_{t} = \mathbf{F}_{D} + \mathbf{F}_{g} + \mathbf{F}_{tp}$$

The drag force ${\bm F}_D$ is defined using the Stokes drag law,

$$\mathbf{F}_{\mathrm{D}} = \left(\frac{1}{\tau_{\mathrm{p}}}\right) m_{\mathrm{p}}(\mathbf{u} - \mathbf{v})$$

where **u** and **v** are the fluid and particle velocity, respectively (SI unit: m/s). The particle velocity response time τ_p (SI unit: s) is a measure of the time scale for the particle velocity to approach that of the surrounding fluid. For the Stokes drag law,

$$\tau_{\rm p} = \frac{\rho_{\rm p} d_{\rm p}^2}{18\mu}$$

where

- μ is the fluid dynamic viscosity (SI unit: Pa s),
- ρ_p is the particle density (SI unit: kg/m³), and
- d_p is the particle diameter (SI unit: m).

The Stokes drag law is applicable when the particles are sufficiently small and move slowly relative to the surrounding fluid. For large, heavy particles with more inertia, an alternative formulation like the Schiller-Naumann drag law might be more appropriate.

GRAVITY FORCE

The **Gravity Force** node also includes the buoyancy force by considering the density of the surrounding fluid ρ (SI unit: kg/m³). The gravity force, **F**_g, is thus

$$\mathbf{F}_{g} = m_{p} \mathbf{g} \frac{(\rho_{p} - \rho)}{\rho_{p}}$$

THERMOPHORETIC FORCE

The **Thermophoretic Force** applies to particles in a nonisothermal flow. The driving mechanism behind this force is the collision of gas molecules on the particle surface. Collisions are more likely to occur on the hotter side of the particle where the average molecular velocity of the gas is greater. This results in a net force toward colder regions of the gas.

In a continuum flow, the thermophoretic force, \mathbf{F}_{tp} , is defined as

$$\mathbf{F}_{\rm tp} = -\frac{6\pi d_{\rm p}\mu^2 C_{\rm s}\Lambda\nabla T}{\rho(2\Lambda+1)T}$$
$$\Lambda = \frac{k}{k_{\rm p}}$$

where

- *k* (SI unit: W/(m K)) is the thermal conductivity of the fluid,
- k_p (SI unit: W/(m K)) is the particle thermal conductivity,
- T (SI unit: K) is the fluid temperature,
- d_{p} (SI unit: m) is the particle diameter,
- ρ (SI unit: kg/m³) is the fluid density, and
- $C_{\rm s}$ is a dimensionless constant equal to 1.17.

The **Thermophoretic Force** node also provides some corrections for high Knudsen number flows, when the mean free path between gas molecule collisions is comparable in size to the particle diameter. However, in the present model, such high Knudsen number corrections can safely be neglected.

Results and Discussion

The gas velocity is plotted in Figure 2 and the temperature in Figure 3. The gas velocity is higher at the outlet than at the inlet due to thermal expansion. The strong heating of the gas by the susceptor causes a decrease in density, so the gas velocity must increase in order for the total mass in the system to be conserved.

The particles begin to move from left to right due to the drag force and also vertically due to the thermophoretic force; see Figure 4. The color of the particle trajectories represents the magnitude of the thermophoretic force. This is because the susceptor temperature is higher than the temperature on the upper surface. The more the temperature of the susceptor increases, the larger the particle free zone which develops just above. The height of the particle-free zone versus the susceptor temperature is plotted in Figure 5 and agrees well with Fig 6a in Ref. 1. The height of the particle-free zone clearly increases as the susceptor temperature increases, indicating an increase in the magnitude of the thermophoretic force.

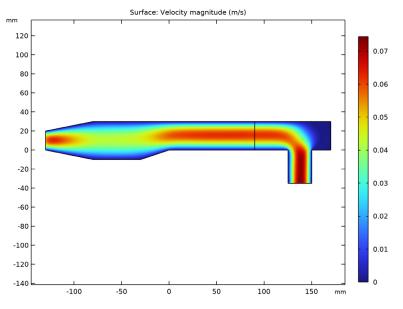


Figure 2: Velocity magnitude.

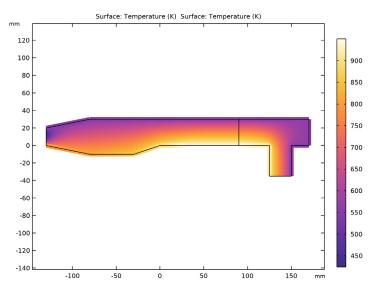


Figure 3: Temperature inside the reactor.

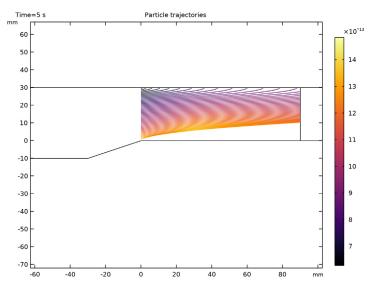


Figure 4: Particle trajectories as they pass over the heated surface.

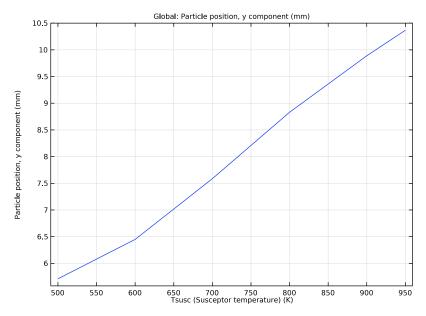


Figure 5: Minimum height of the particles versus temperature.

Notes About the COMSOL Implementation

The model is solved in two stages. First, the gas velocity, pressure, and temperature are computed using a **Stationary** study. Next, the Particle Tracing for Fluid Flow interface is added to the model and the trajectories are computed in a separate **Time Dependent** study. Finally, a **Parametric Sweep** is added with two study steps, a **Stationary** step for the gas flow, followed by a **Time Dependent** step for the particle trajectories. The parametric sweep is performed for a range of susceptor surface temperatures, meaning that both the gas flow and particle trajectories need to be recomputed for each parameter value.

Reference

1. Dimitrios I. Fotiadis, and Klavs F. Jensen, "Thermophoresis of solid particles in horizontal chemical vapor deposition reactors," *J. Crystal Growth*, vol. 102 pp 743–761, 1990.

Application Library path: CFD_Module/Particle_Tracing/thermophoresis

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click 🔗 Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click **Q** 2D.
- 2 In the Select Physics tree, select Fluid Flow>Nonisothermal Flow>Laminar Flow.
- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select General Studies>Stationary.
- 6 Click **M** Done.

GEOMETRY I

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose mm.

Rectangle 1 (r1)

- I 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 170.
- 4 In the **Height** text field, type 30.

Line Segment I (Is I)

- I In the Geometry toolbar, click 😕 More Primitives and choose Line Segment.
- 2 In the Settings window for Line Segment, locate the Starting Point section.
- **3** From the **Specify** list, choose **Coordinates**.
- 4 Locate the Endpoint section. From the Specify list, choose Coordinates.
- 5 Locate the Starting Point section. In the x text field, type 30.

6 Locate the **Endpoint** section. In the **x** text field, type 90.

Rectangle 2 (r2)

- I 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 50.
- **4** In the **Height** text field, type **40**.
- 5 Locate the **Position** section. In the **x** text field, type -80.
- **6** In the **y** text field, type -10.

Polygon I (poll)

- I In the **Geometry** toolbar, click **/ Polygon**.
- 2 In the Settings window for Polygon, locate the Coordinates section.
- **3** From the **Data source** list, choose **Vectors**.
- 4 In the x text field, type -30 30 30 0 0 -10 -10 30.
- **5** In the **y** text field, type 30 30 30 0 0 -10 -10 30.
- 6 In the x text field, type -30 0 0 0 0 -30 -30 -30.

Polygon 2 (pol2)

- I In the Geometry toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Coordinates section.
- 3 From the Data source list, choose Vectors.
- 4 In the x text field, type -80 -130 -130 -130 -130 -80 -80.
- 5 In the y text field, type 30 20 20 0 0 -10 -10 30.

Line Segment 2 (Is2)

- I In the Geometry toolbar, click 😕 More Primitives and choose Line Segment.
- 2 In the Settings window for Line Segment, locate the Starting Point section.
- **3** From the **Specify** list, choose **Coordinates**.
- 4 Locate the Endpoint section. From the Specify list, choose Coordinates.
- 5 Locate the Starting Point section. In the x text field, type 90.
- 6 Locate the **Endpoint** section. In the **x** text field, type 90.
- 7 In the y text field, type 30.

Rectangle 3 (r3)

I 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 25.
- 4 In the **Height** text field, type 35.
- 5 Locate the **Position** section. In the **x** text field, type 125.
- 6 In the y text field, type -35.

Union I (uni I)

- I In the Geometry toolbar, click i Booleans and Partitions and choose Union.
- 2 Select the objects poll, pol2, rl, r2, and r3 only.
- 3 In the Settings window for Union, locate the Union section.
- **4** Clear the **Keep interior boundaries** check box.

Form Union (fin)

- I In the Geometry toolbar, click 🟢 Build All.
- 2 Click the **Zoom Extents** button in the **Graphics** toolbar.

GLOBAL DEFINITIONS

Parameters 1

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

- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
Tsusc	950[K]	950 K	Susceptor temperature
d_part	2e-6[m]	2E-6 m	Particle diameter
rho_part	2200[kg/m^3]	2200 kg/m ³	Particle density
depth	74[mm]	0.074 m	Model depth

DEFINITIONS

Walls

- I In the Model Builder window, expand the Component I (compl)>Definitions node.
- 2 Right-click **Definitions** and choose **Selections>Explicit**.
- 3 In the Settings window for Explicit, type Walls in the Label text field.
- 4 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- **5** Select Boundaries 2–9, 12–14, and 16–18 only.

ADD MATERIAL

- I In the Home toolbar, click 🙀 Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Liquids and Gases>Gases>Hydrogen.
- 4 Click Add to Component in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Material to close the Add Material window.

HEAT TRANSFER IN FLUIDS (HT)

Temperature 1

- I In the Model Builder window, under Component I (compl) right-click Heat Transfer in Fluids (ht) and choose Temperature.
- **2** Select Boundary 10 only.
- 3 In the Settings window for Temperature, locate the Temperature section.
- **4** In the T_0 text field, type Tsusc.

Inflow I

- I In the Physics toolbar, click Boundaries and choose Inflow.
- 2 Select Boundary 1 only.
- 3 In the Settings window for Inflow, locate the Upstream Properties section.
- 4 In the $T_{\rm ustr}$ text field, type 300.

Outflow I

- I In the Physics toolbar, click Boundaries and choose Outflow.
- 2 Select Boundary 15 only.

LAMINAR FLOW (SPF)

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

- I In the Model Builder window, under Component I (compl) click Laminar Flow (spf).
- 2 In the Settings window for Laminar Flow, locate the Physical Model section.
- 3 From the Compressibility list, choose Compressible flow (Ma<0.3).

Inlet 1

- I 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 Mass flow.
- 5 Locate the Mass Flow section. From the Mass flow type list, choose Standard flow rate (SCCM).
- **6** In the Q_{sccm} text field, type 2000.
- 7 In the M_n text field, type 0.002.
- 8 In the $d_{\rm bc}$ text field, type depth.

Outlet I

- I In the Physics toolbar, click Boundaries and choose Outlet.
- **2** Select Boundary 15 only.

HEAT TRANSFER IN FLUIDS (HT)

In the Model Builder window, under Component I (compl) click Heat Transfer in Fluids (ht).

Heat Flux 1

- I In the Physics toolbar, click Boundaries and choose Heat Flux.
- 2 In the Settings window for Heat Flux, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- 4 Locate the Heat Flux section. From the Flux type list, choose Convective heat flux.
- **5** In the h text field, type 10.

Thin Layer I

- I In the Physics toolbar, click Boundaries and choose Thin Layer.
- 2 In the Settings window for Thin Layer, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- 4 Locate the Layer Model section. From the Layer type list, choose

Thermally thin approximation.

Since the **Thin Layer** feature has been added, material properties need to be defined on those boundaries.

MATERIALS

Material 2 (mat2)

- I In the Model Builder window, under Component I (comp1) right-click Materials and choose Layers>Single Layer Material.
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.

3 From the Selection list, choose Walls.

4 Locate the Material Contents section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Heat capacity at constant pressure	Ср	800	J/(kg·K)	Basic
Density	rho	2700	kg/m³	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	160	W/(m·K)	Basic
Thickness	lth	5[mm]	m	Shell

MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Physics-Controlled Mesh section.
- **3** From the **Element size** list, choose **Fine**.
- 4 Click 📗 Build All.

STUDY I

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

The default plots which are created automatically are a surface plot of the velocity field (Figure 2), a contour plot of the pressure, a surface temperature plot (Figure 3), and a contour plot of the temperature.

RESULTS

Velocity (spf)

Next, set up the Particle Tracing Interface.

ADD PHYSICS

- I In the Home toolbar, click 🙀 Add Physics to open the Add Physics window.
- **2** Go to the **Add Physics** window.
- 3 In the tree, select Fluid Flow>Particle Tracing>Particle Tracing for Fluid Flow (fpt).
- 4 Click Add to Component I in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Physics to close the Add Physics window.

ADD STUDY

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

PARTICLE TRACING FOR FLUID FLOW (FPT)

In the Model Builder window, under Component I (compl) click Particle Tracing for Fluid Flow (fpt).

Drag Force 1

- I In the Physics toolbar, click **Domains** and choose **Drag Force**.
- 2 In the Settings window for Drag Force, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.
- 4 Locate the Drag Force section. From the u list, choose Velocity field (spf).
- **5** From the μ list, choose **Dynamic viscosity (spf)**.
- 6 Locate the Model Input section. From the T list, choose Temperature (ht).
- **7** From the p_A list, choose **Absolute pressure (spf)**.

Thermophoretic Force 1

- I In the Physics toolbar, click 🔵 Domains and choose Thermophoretic Force.
- 2 In the Settings window for Thermophoretic Force, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.
- 4 Locate the Fluid Properties section. From the μ list, choose Dynamic viscosity (spf).
- **5** From the ρ list, choose **Density (spf)**.
- 6 Locate the Advanced Settings section. Select the Use piecewise polynomial recovery on field check box.
- 7 Locate the Model Input section. From the T list, choose Temperature (ht).
- **8** From the p_A list, choose **Absolute pressure (spf)**.

Wall 2

- I In the Physics toolbar, click Boundaries and choose Wall.
- 2 Select Boundary 11 only.

Gravity Force 1

- I In the Physics toolbar, click **Domains** and choose Gravity Force.
- 2 In the Settings window for Gravity Force, locate the Domain Selection section.
- 3 From the Selection list, choose All domains.
- **4** Locate the **Gravity Force** section. From the ρ list, choose **Density (spf)**.

Release from Grid I

- I In the Physics toolbar, click 🖗 Global and choose Release from Grid.
- 2 In the Settings window for Release from Grid, locate the Initial Coordinates section.
- 3 Click Y Range.
- 4 In the Range dialog box, choose Number of values from the Entry method list.
- 5 In the Start text field, type 0.01.
- 6 In the Stop text field, type 29.99.
- 7 In the Number of values text field, type 50.
- 8 Click Replace.
- 9 In the Settings window for Release from Grid, locate the Initial Velocity section.
- **IO** Specify the \mathbf{v}_0 vector as

u x

v y

Particle Properties 1

- I In the Model Builder window, click Particle Properties I.
- 2 In the Settings window for Particle Properties, locate the Particle Properties section.
- 3 From the ρ_p list, choose User defined. In the associated text field, type rho_part.
- **4** In the d_p text field, type d_part.
- 5 Locate the Additional Material Properties section. From the k_p list, choose User defined. In the associated text field, type 1.38.

STUDY 2

Step 1: Time Dependent

- I In the Model Builder window, under Study 2 click Step I: Time Dependent.
- 2 In the Settings window for Time Dependent, locate the Study Settings section.
- 3 Click Range.

- 4 In the Range dialog box, choose Number of values from the Entry method list.
- 5 In the **Stop** text field, type 5.
- 6 In the Number of values text field, type 50.
- 7 Click Replace.
- 8 In the Settings window for Time Dependent, locate the Physics and Variables Selection section.
- 9 Select the Modify model configuration for study step check box.
- 10 In the tree, select Component 1 (comp1)>Laminar Flow (spf).
- II Click (**Disable in Solvers**.
- 12 In the tree, select Component I (compl)>Heat Transfer in Fluids (ht).
- **I3** Click (**Disable in Solvers**.
- 14 In the tree, select Component I (compl)>Multiphysics>Nonisothermal Flow I (nitfl).
- **I5** Click (**Disable in Solvers**.
- 16 Click to expand the Values of Dependent Variables section. Find the Values of variables not solved for subsection. From the Settings list, choose User controlled.
- **I7** From the **Method** list, choose **Solution**.
- 18 From the Study list, choose Study 1, Stationary.
- **19** In the **Home** toolbar, click **= Compute**.

RESULTS

Particle Trajectories (fpt)

- I Click the **Zoom Extents** button in the **Graphics** toolbar.
- 2 In the Model Builder window, expand the Particle Trajectories (fpt) node.

Particle Trajectories 1

- In the Model Builder window, expand the Results>Particle Trajectories (fpt)>
 Particle Trajectories I node, then click Particle Trajectories I.
- 2 In the Settings window for Particle Trajectories, locate the Coloring and Style section.
- 3 Find the Line style subsection. From the Type list, choose Line.
- 4 Find the **Point style** subsection. From the **Type** list, choose **None**.
- 5 In the Particle Trajectories (fpt) toolbar, click **O** Plot.

Color Expression 1

- I In the Model Builder window, click Color Expression I.
- 2 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Particle Tracing for Fluid Flow>Forces>Thermophoretic force N>fpt.thpfl.Ftfy Thermophoretic force, y component.
- 3 Locate the Coloring and Style section. Click Change Color Table.
- 4 In the Color Table dialog box, select Thermal>Inferno in the tree.
- 5 Click OK.
- 6 In the Particle Trajectories (fpt) toolbar, click 💿 Plot.

ADD STUDY

- I In the Home toolbar, click $\sim\sim$ Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Preset Studies for Some Physics Interfaces>Stationary.
- 4 Click Add Study in the window toolbar.
- 5 In the Home toolbar, click 2 Add Study to close the Add Study window.

STUDY 3

Time Dependent

- I In the Study toolbar, click Study Steps and choose Time Dependent> Time Dependent.
- 2 In the Settings window for Time Dependent, locate the Physics and Variables Selection section.
- **3** Select the Modify model configuration for study step check box.
- 4 In the tree, select Component I (compl)>Laminar Flow (spf).
- 5 Click (**)** Disable in Solvers.
- 6 In the tree, select Component I (compl)>Heat Transfer in Fluids (ht).
- 7 Click (**Disable in Solvers**.
- 8 In the tree, select Component I (compl)>Multiphysics>Nonisothermal Flow I (nitfl).
- 9 Click () Disable in Solvers.

10 Locate the Values of Dependent Variables section. Find the

Values of variables not solved for subsection. From the Settings list, choose User controlled.

- II From the Method list, choose Solution.
- 12 From the Study list, choose Study 3, Stationary.
- 13 Locate the Study Settings section. Click Range.
- 14 In the Range dialog box, choose Number of values from the Entry method list.
- **I5** In the **Stop** text field, type **5**.
- **I6** In the **Number of values** text field, type **10**.

17 Click Replace.

Parametric Sweep

- I In the Study toolbar, click **Parametric Sweep**.
- 2 In the Settings window for Parametric Sweep, locate the Study Settings section.
- 3 Click + Add.
- **4** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Tsusc (Susceptor temperature)	500 600 700 800 900 950	К

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

RESULTS

Particle 3

- I In the Model Builder window, expand the Results>Datasets node.
- 2 Right-click Results>Datasets>Particle 2 and choose Duplicate.

Selection

- I In the Results toolbar, click 🖣 Attributes and choose Selection.
- 2 In the Settings window for Selection, locate the Geometric Entity Selection section.
- **3** From the Geometric entity level list, choose Boundary.
- **4** Select Boundary 11 only.

Minimum I

- I In the **Results** toolbar, click **More Datasets** and choose **Evaluation>Minimum**.
- 2 In the Settings window for Minimum, locate the Data section.

- **3** From the **Dataset** list, choose **Particle 3**.
- 4 Locate the Settings section. From the Geometry level list, choose Point.

Particle Position

- I In the **Results** toolbar, click \sim **ID Plot Group**.
- **2** In the **Settings** window for **ID Plot Group**, type **Particle Position** in the **Label** text field.
- 3 Locate the Data section. From the Dataset list, choose Minimum I.
- **4** From the **Time selection** list, choose **Last**.

Global I

- I Right-click Particle Position and choose Global.
- 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 I (compl)>
 Particle Tracing for Fluid Flow>Particle position>qy Particle position, y component m.
- 3 Locate the x-Axis Data section. From the Axis source data list, choose Outer solutions.
- **4** In the **Particle Position** toolbar, click **I Plot**.
- 5 Click to expand the Legends section. Clear the Show legends check box.