Model created in COMSOL Multiphysics 6.4

Convective Evaporation of a Water–Acetone Droplet

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Introduction

In this model the evaporation of a water-acetone droplet on a marble substrate is studied in detail. The droplet consists of a concentrated aqueous solution that initially contains 20% acetone by weight. The model describes the coupled phenomena of mass and heat transfer across the vapor–liquid interface, and accounts for multiphase flow by solving for the velocity in both the vapor and the liquid. As the droplet evaporates, the model tracks the position of the vapor–liquid interface.

Practical applications where detailed modeling of evaporation is valuable are found over a wide range of industries such as the pharmaceutical industry, fine chemicals production, and other industries where separation and drying processes need to be investigated.

Model Definition

The droplet rests on a marble substrate inside a channel. The droplet is subjected to an impinging gas jet with a specified relative humidity. At the studied conditions, the vapor pressures of acetone and water are higher than that of the impinging jet. This results in evaporation of both species. The evaporation is accelerated by the gas jet which transports vapor along the droplet surface and subsequently away from the droplet. The heat of evaporation is included, giving a decrease in the droplet temperature during evaporation. Due to its higher vapor pressure, acetone evaporates faster than water. This results in a change in acetone concentration over time. The droplet decreases in size until most of the acetone has evaporated from the droplet. When mainly water remains, the evaporation continues at a lower rate.

The model setup including the inlet and initial conditions are seen in is seen in Figure 1. As the system is symmetric a 2D axially symmetric geometry is used. The droplet surface is modeled as being infinitely thin and represented as an interior boundary on a moving mesh. In order to refine the mesh just outside and below the droplet, two interior boundaries seen in Figure 2 are included. This also allows for solving for the mesh only in the droplet and the vapor domain next to it, keeping the mesh fixed in the rest of the geometry. These extra interior boundaries are not part of the physical geometry and are hidden when evaluating the results.

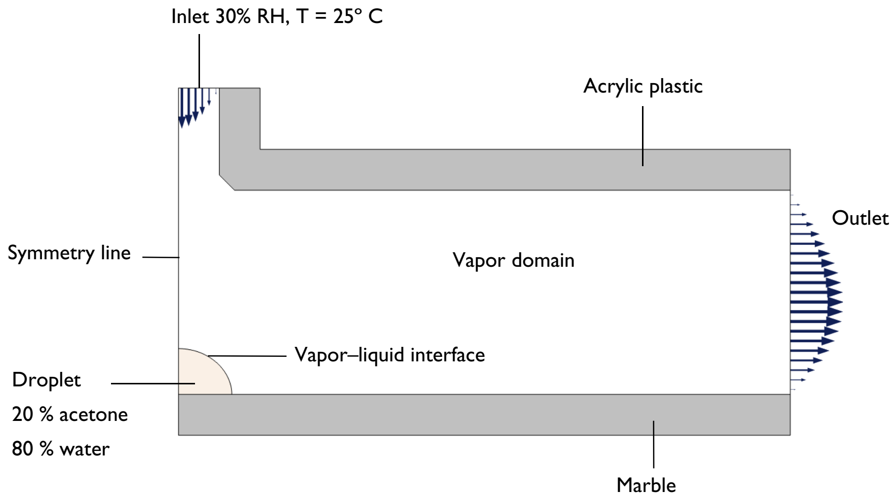

Figure 1: The droplet and channel geometry including the system conditions.

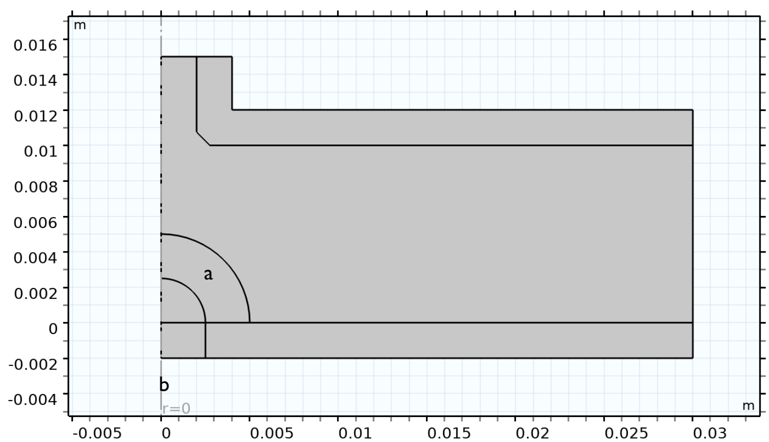

Figure 2: The model geometry includes two interior boundaries, indicated "a" and "b", which are used to refine the mesh in the vicinity of the droplet.

COMSOL IMPLEMENTATION

The current model is built by combining functionality for vapor–liquid equilibria, fluid flow, heat transfer, and moving mesh. A **Transport of Concentrated Species in Vapor** interface is used to solve for the mass transport in both the vapor and the droplet. It includes a **Vapor–Liquid-Mixture Interface** feature prescribing vapor–liquid equilibrium conditions at the droplet surface. Functions for the vapor pressures, obtained using a **Thermodynamic System** feature, accounts for the temperature, pressure, and liquid composition along the droplet surface. A **Laminar Flow** interface is used to solve for the fluid flow in the vapor and the droplet. It includes a **Fluid-Fluid Interface** feature which, together with a **Moving Mesh** interface, tracks the droplet surface position as it moves due to the evaporative mass transfer. A constant **Contact Angle** is used, but the contact angle can also be an expression that varies with concentration or time. Finally, a **Heat Transfer in Fluids** interface is used to solve for the temperature in the vapor, liquid, and the channel structure, including the substrate on which the droplet rests. Composition-dependent properties are used both in the vapor and in the liquid. The equations and boundary conditions used are described in the sections below.

CHEMISTRY AND THERMODYNAMICS

The **Chemistry** interface defines properties of the species, and the thermodynamic properties of the gas phase. The chemical species present are water, acetone, and nitrogen. By coupling the chemistry interface to a vapor–liquid **Thermodynamic System**, both the species properties and the gas phase properties are defined from the thermodynamic system. Examples of species properties defined are the molar mass, the thermal conductivity, and the enthalpy of formation. Properties of the gas phase are for example the density, viscosity and heat capacity. The liquid droplet consist of water and acetone. A material feature defining the droplet properties is generated from the vapor–liquid thermodynamic system. Both the gas phase and the liquid phase are modeled as being ideal.

FLUID FLOW

The pressure differences are assumed small and the fluid flow in both phases is defined as weakly compressible meaning that the density of the fluid is evaluated at a reference pressure.

$$\rho = \rho(p_{\mathrm{ref}}, T).$$

This gives the following form of the momentum equations

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mathbf{K}] + \rho g,$$

and the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0.$$

The momentum equations includes gravity, ρg, since this affects the droplet shape. As will be seen in the results, buoyancy drives a circulating flow in the droplet. The buoyancy is caused by both the heat of evaporation and the variation in the composition.

A Navier slip boundary condition is used on the boundary between the shrinking droplet and the solid table. This boundary condition allows the edge of drop to slide along the solid, but also accounts for the tangential wall stress that acts to retard the flow. The drop shrinks due to evaporation. This is modeled by specifying the resulting evaporative mass flux (caused by the vapor–liquid equilibrium) as the mass transfer across the droplet surface.

VAPOR–LIQUID EQUILIBRIUM

To model the evaporation of acetone and water from the droplet, a vapor–liquid equilibrium condition is prescribed at the surface of the droplet. For a solution, thermodynamic equilibrium is reached when the fugacities are the same in both phases (for each species i)

$$f_i^{\mathrm{V}}(T, P, y_i) = f_i^{\mathrm{L}}(T, P, x_i). \tag{1}$$

Here, f_i^V denotes the vapor phase fugacity, and f_i^{L} is the liquid phase fugacity. The fugacity is a measure of the chemical potential and relates to the tendency of a substance to prefer one of the phases over the other. In general, the fugacity in each phase depends on the temperature, T, the absolute pressure, P, as well as composition. The composition is usually expressed by the molar fractions in each phase, y_i and x_i, respectively. When accounting for nonideal behavior, the fugacity equality in Equation 1 can be formulated as (see Ref. 1)

$$\hat{\phi}_i y_i P = \gamma_i x_i \phi_i^{\mathrm{sat}} P_i^{\mathrm{sat}} \exp\left[\int_{P_i^{\mathrm{sat}}}^{P} \frac{V_i^{\mathrm{L}}}{RT} dP\right]. \tag{2}$$

Here the fugacity coefficient $\hat{\phi}_i$ accounts for nonideality in the gas, while the activity coefficient γ_i, accounts for nonideality in the liquid phase. Both these coefficients are functions of the temperature, pressure, and fraction of species i in the respective solutions. For the liquid, ϕ_i^{sat} and P_i^{sat} denote the fugacity coefficient and the vapor pressure, both for a pure species i. The superscript 'sat' indicates saturation conditions. The exponential term on the right hand side is the Poynting correction factor, including the molar liquid volume $V_i^{\mathrm{L}} = M_i / \rho^{\mathrm{L}}$. Here, M_i is the molar mass of species i. The correction factor describes the effect of pressure on the liquid fugacity. For low pressures, the Poynting correction factor is close to one, and two simplified relations can be formulated.

- In the case of an ideal gas mixture and an ideal liquid solution, the fugacity coefficient and the activity coefficient are both one, and Equation 2 reduces to Raoult's law:

$$y_i P = x_i P_i^{\mathrm{sat}} \tag{3}$$

- For an ideal gas mixture, but a nonideal liquid solution, Equation 2 reduces to the modified Raoult's law:

$$y_i P = \gamma_i x_i P_i^{\mathrm{sat}}. \tag{4}$$

Assuming that the thermodynamic equilibrium prevails at the vapor–liquid interface, the molar fraction to prescribe on the vapor side of the interface is in general (from Equation 2)

$$y_i = \frac{f_i^{\mathrm{L}}(T, P, x_i)}{\hat{\phi}_i(T, P, y_i)P}. \tag{5}$$

The **Vapor–Liquid-Mixture Interface** feature used in this model introduces separate composition variables for the two phases along the droplet surface. To enforce a thermodynamic equilibrium, the composition on the vapor side is prescribed from Equation 5 using the liquid composition, the temperature, and the pressure at the surface. When the feature is coupled to a thermodynamics system, functions for both the liquid phase fugacity, and the vapor phase fugacity are available.

In the **Vapor–Liquid-Mixture Interface** feature it is also possible to prescribe a vapor pressure for each species. In this case, the system is assumed ideal and the vapor molar fraction is

$$y_i = \frac{x_i P_i^{\mathrm{sat}}}{P}. \tag{6}$$

The **Transport of Concentrated Species in Vapor** interface solves for the mass fractions ω. The boundary condition applied on the vapor side of the droplet surface is for species i

$$\omega_i^{\mathrm{V}} = \frac{y_i M_i}{M_{\mathrm{n}}^{\mathrm{V}}} = \frac{x_i P_i^{\mathrm{sat}}}{P}\frac{M_i}{M_{\mathrm{n}}^{\mathrm{V}}}, \tag{7}$$

where $M^{\mathrm{V}}{}_{\mathrm{n}}$ is the mean molar mass of the vapor.

Using the ideal gas law of the form

$$P = \frac{\rho^{\mathrm{V}} RT}{M_{\mathrm{n}}^{\mathrm{V}}}, \tag{8}$$

the vapor side concentration corresponds to

$$c_i^{\mathrm{V}} = \frac{\omega_i^{\mathrm{V}} \rho^{\mathrm{V}}}{M_i} = \frac{x_i P_i^{\mathrm{sat}}}{P} \frac{\rho^{\mathrm{V}}}{M_n^{\mathrm{V}}} = \frac{x_i P_i^{\mathrm{sat}}}{PT}. \tag{9}$$

MODELING EVAPORATION

In this model example, the acetone and water mass fractions are prescribed on the vapor side of the droplet surface according to Equation 7. This results in a mass flux of each species through the phase boundary. As the acetone concentration in the vapor is initially zero, acetone is transported from the liquid surface into the vapor phase. As the vapor pressure of water at the surface is higher than the ambient vapor pressure, water also evaporates from the droplet. In cases where the droplet vapor pressure decreases below the ambient pressure, for example due to a decrease in temperature, vapor will instead condense at the droplet surface.

The total vapor mass flux (kg/(m²·s)) across the droplet surface corresponds to the sum of the water and acetone mass fluxes in the vapor

$$j^{\mathrm{V}} = j_{\mathrm{w}}^{\mathrm{V}} + j_{\mathrm{a}}^{\mathrm{V}} = \mathbf{n} \cdot (\mathbf{j}_{\mathrm{w}}^{\mathrm{V}} + \rho^{\mathrm{V}} \mathbf{u}^{\mathrm{V}} \omega_{\mathrm{w}}^{\mathrm{V}}) + \mathbf{n} \cdot (\mathbf{j}_{\mathrm{a}}^{\mathrm{V}} + \rho^{\mathrm{V}} \mathbf{u}^{\mathrm{V}} \omega_{\mathrm{a}}^{\mathrm{V}}). \tag{10}$$

Here, $\mathbf{j}^{\mathrm{V}}_{\mathrm{w}}$ and $\mathbf{j}^{\mathrm{V}}_{\mathrm{a}}$ denote the diffusive mass transfer in the vapor, resulting from enforcing the equilibrium conditions in Equation 7, and $\mathbf{n}$ is the surface normal. It can be noted that the total mass flux corresponds to an equivalent Stefan velocity for the vapor phase

$$j^{\mathrm{V}} = \rho^{\mathrm{V}} u_{\mathrm{s}}^{\mathrm{V}}. \tag{11}$$

To conserve mass during phase transfer, the normal mass flux on the liquid side must be equal to the normal mass flux of vapor from the phase boundary. The normal diffusive mass fluxes on the liquid side are thus defined as

$$\begin{aligned} \mathbf{n} \cdot \mathbf{j}_{\mathrm{w}}^{\mathrm{L}} &= j^{\mathrm{V}} (\omega_{\mathrm{w}}^{\mathrm{L}} - \omega_{\mathrm{w}}^{\mathrm{V}}) \\ \mathbf{n} \cdot \mathbf{j}_{\mathrm{a}}^{\mathrm{L}} &= j^{\mathrm{V}} (\omega_{\mathrm{a}}^{\mathrm{L}} - \omega_{\mathrm{a}}^{\mathrm{V}}) \end{aligned}, \tag{12}$$

to enforce that the mass fraction on the liquid side is adjusted with the corresponding evaporating mass fraction

$$\omega_i^V = \frac{j_i^V}{j^V}. \tag{13}$$

The **Fluid-Fluid Interface** feature in the **Laminar Flow** interface specifies boundary conditions for the fluid flow at the droplet surface. It includes surface tension and describes the velocity of the phase boundary in combination with the **Moving Mesh** interface. Similar to the corresponding feature for mass transfer, the **Fluid-Fluid Interface** feature introduces separate velocity and pressure variables in the vapor and the liquid.

The relationship governing the velocities of the vapor and the liquid at the surface is

$$\mathbf{u}^L = \mathbf{u}^V + j^V\left(\frac{1}{\rho^L} - \frac{1}{\rho^V}\right)\mathbf{n}, \tag{14}$$

where the mass transfer across the interface corresponds to the total vapor mass flux j^V. It can be noted that a nonzero mass flux is necessary for the phase velocities to differ. The difference is prescribed in the normal direction of the surface. Furthermore, if the densities of both phases are the same, the phase velocities are also identical.

The relationship between the mesh velocity and the liquid velocity is

$$\mathbf{u}_{mesh} \cdot \mathbf{n} = \left(\mathbf{u}^L - \frac{j^V}{\rho^L}\right)\mathbf{n}. \tag{15}$$

The mesh velocity is the velocity of the fluid-fluid interface. In a situation without evaporation, the normal mesh velocity equals the normal liquid velocity. For a non-zero mass flux on the other hand, the surface normal mesh velocity differs from that of the liquid phase.

The heat of evaporation at the fluid-fluid interface (W/m^2) is defined as

$$Q_{vap} = j_w^V \Delta H_{vap,w} + j_a^V \Delta H_{vap,a}. \tag{16}$$

Here, j^V_i is the normal mass flux across the liquid surface for species i (acetone or water) from Equation 7, and $\Delta H_{vap,i}$ is the species heat of evaporation (J/kg). When coupled to a thermodynamic system, functions for the heat of evaporation are added automatically. The resulting heat of evaporation is defined by the **Vapor–Liquid-Mixture Interface** feature. This heat source is then applied to the droplet surface using a **Boundary Heat Source** feature in the **Heat Transfer in Fluids** interface.

This model contains two studies. The first study is used to initialize the droplet shape. Here, the fluid flow and moving mesh are solved for. Gravity, surface tension, and the flowing gas will affect the droplet shape.

The second study solves for the evaporation process. Figure 3 illustrates the fluid velocity at four different times, both in the droplet and in the vapor. The change in droplet size due to evaporation is also visible.

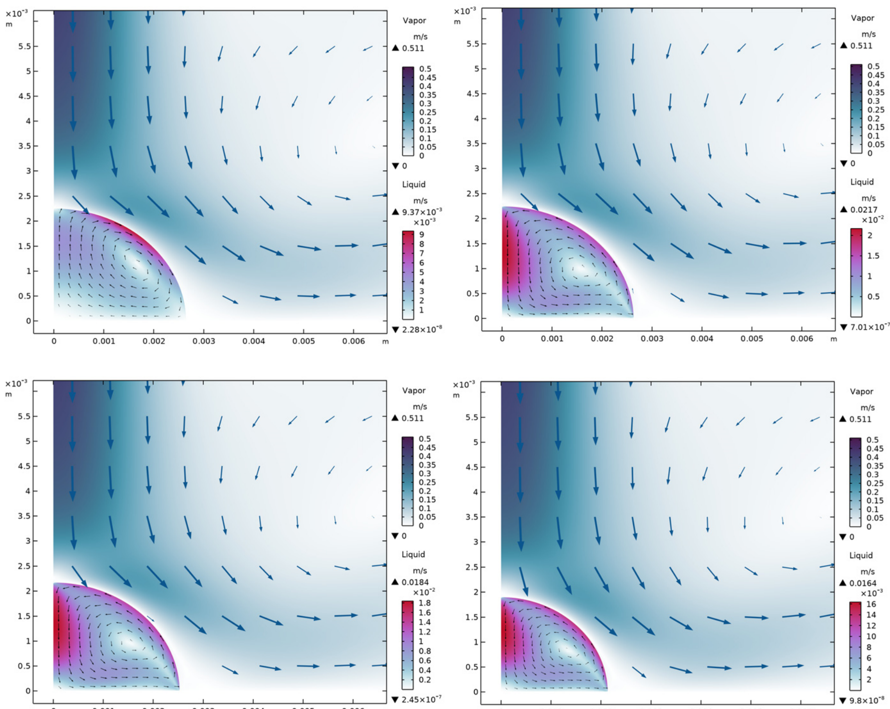

Figure 3: Velocity in the vapor and the liquid droplet at t = 0 s (upper left), t = 10 s (upper right), t = 100 s (lower left), and t = 1000 s (lower right).

The vapor phase flow is not varying with time, but the droplet flow velocity goes through some interesting phases. Initially, the liquid is moving in clockwise direction due to the shear stress from the vapor flow. After 0.5 s, the flow begins to change direction, starting at the edge of the drop resting on the table. This flow reversal process lasts for approximately one second. After this, the flow field does not change significantly, but the velocity decreases with decreased acetone concentration. The flow field direction inside the droplet results from the density gradient in the drop during the evaporation. Figure 4 illustrates the density in the system after 60 s.

As acetone evaporates, the density of the liquid increases. The evaporative mass flux is highest close the droplet top, since the driving force is highest here. The high driving force at the top is a result of two things. Firstly the vapor flow rate is at its highest here, and secondly, the low concentration of upstream acetone. The density in the liquid will increase the most at this position, creating a downward flow of liquid in the center of the drop, as seen in Figure 3.

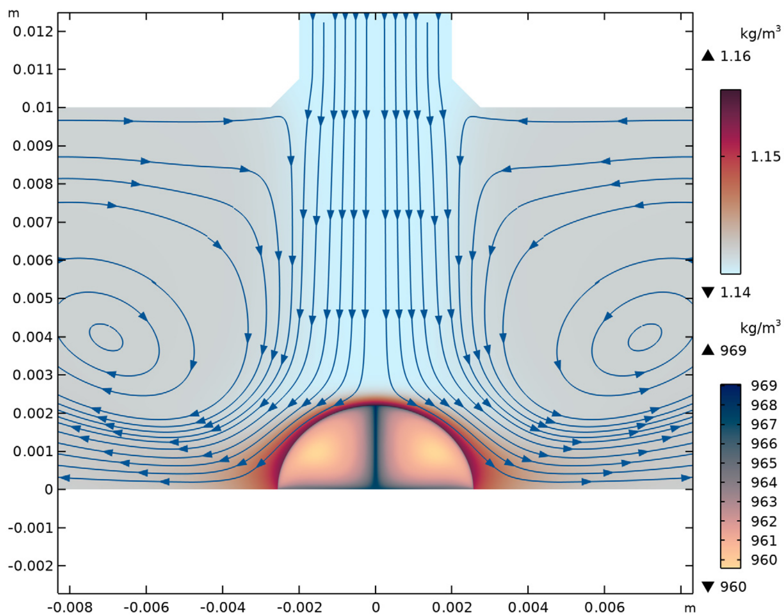

Figure 4: Vapor and liquid density after 60 s.

The decrease in temperature due to evaporation increases the liquid density further as it passes along the surface. The temperature in the system after 60 s is seen in Figure 5.

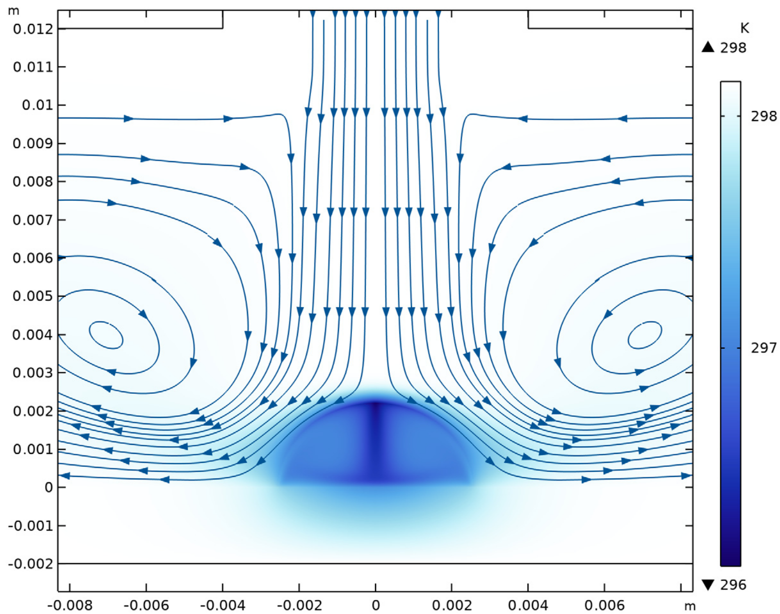

Figure 5: The temperature in the system after 60 s.

Initially the vapor phase surrounding the droplet is free from acetone, and the droplet has no concentration gradients. Figure 6 illustrates the partial pressure, and molar concentration of acetone in the system after 60 s. The acetone concentration in the liquid close to the surface decreases due to phase transfer to the surrounding vapor. The low diffusion rate in the liquid causes sharp gradients. The acetone-free vapor flow from above increases the evaporation rate and prevents an equilibrium. As a consequence, the drop will eventually consist of pure water. The comparatively thin boundary layer on the vapor side, at the droplet top, is a result of the flow of vapor.

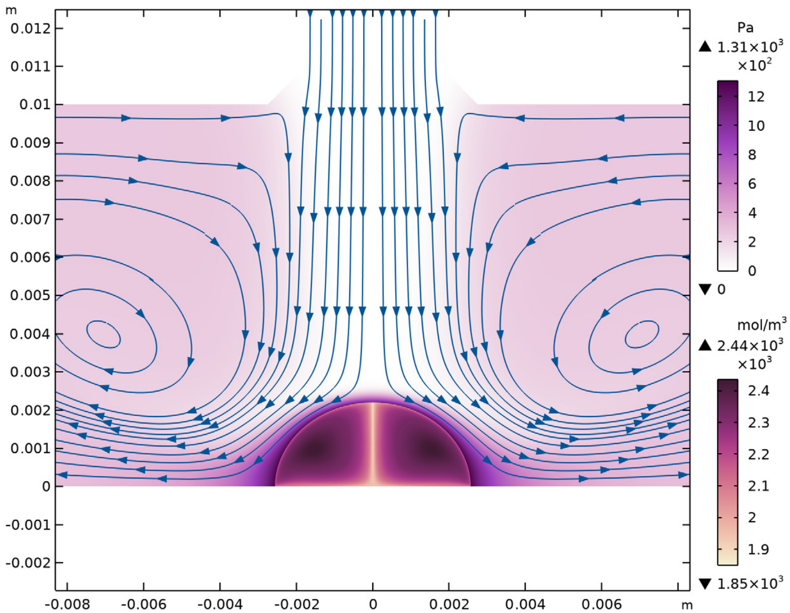

Figure 6: Acetone vapor pressure and concentration, together with vapor velocity streamlines after 60 s of evaporation.

The water vapor pressure and concentration at 60 s is seen in Figure 7. The concentration of water in the liquid is increased at the surface of the droplet due to the higher evaporation rate of acetone.

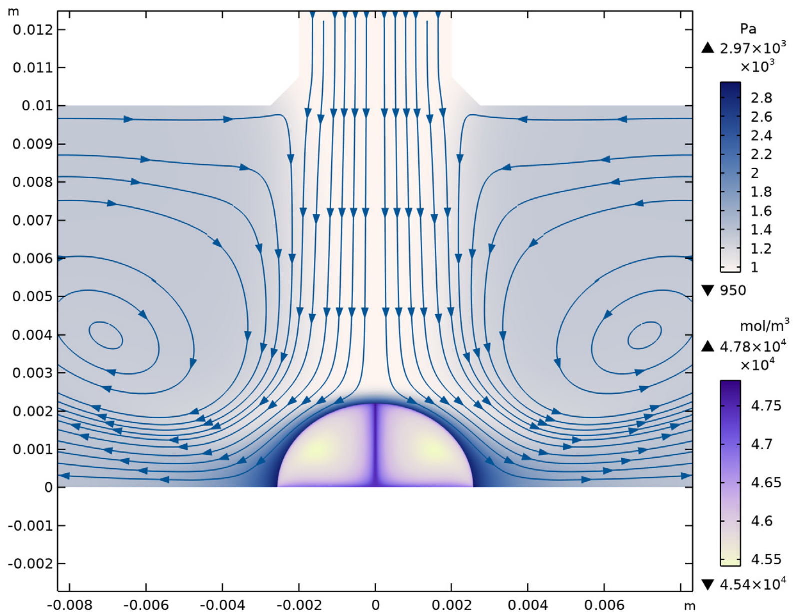

Figure 7: Water vapor pressure and concentration, together with vapor velocity streamlines after 60 s of evaporation.

The total evaporation rate along the fluid-fluid interface, the droplet temperature at two positions, and the total droplet shrinkage over time is illustrated in Figure 8.

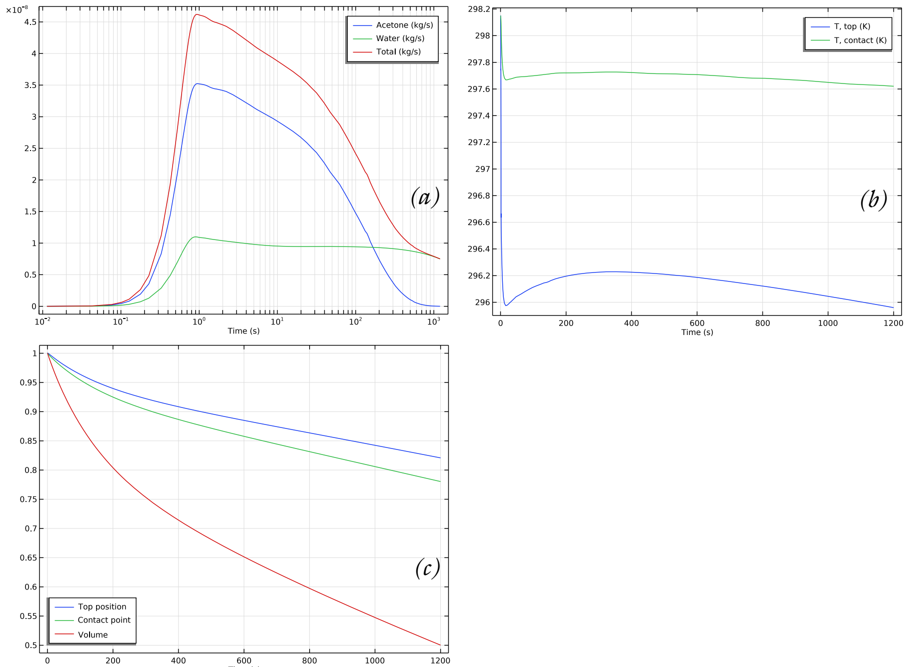

Figure 8: (a) Total evaporation rates for each species along the fluid-fluid interface, (b) the temperature at the top and edge of the droplet, and (c) the shrinkage of the droplet over time.

Figure 8 (a) shows that the evaporation rate is reaching a maximum after a few seconds. Initially, the gas phase is free from acetone, and the concentration in the droplet is homogeneous, giving a maximum evaporation rate. After time, the concentration of acetone in the liquid close to the surface is depleted, and the partial pressure of acetone is significant. These two factors, together with the decrease in temperature, decrease the driving force, and thus the evaporation rate. When the evaporation rate decreases, the temperature of the drop increases slightly, before decreasing again, as seen in Figure 8 (b). Figure 8 (c) shows that the drop volume is reduced to half its original volume during the time studied.

Notes About the COMSOL Implementation

The geometry is united using the **Form Assembly** method. This is used to introduce different meshes at the droplet bottom and top the solid under it, such that the droplet surface can slide along the solid. The identity pairs needed to connect the domains and get a continuous temperature field are added automatically. For efficiency, the mesh is only solved for in the droplet domain and the small vapor domain adjacent to it.

The model includes two studies. The first study is used to initialize the droplet shape. Here, only the fluid flow and moving mesh are solved for. The gravity is introduced gradually over time. This is done to progress the droplet smoothly from the initial circular shape to the shape where the droplet weight is balanced by surface tension.

In the second step the droplet shape is initialized from the first study, and evaporation is modeled by solving for all coupled physics interfaces as well as tracking the interface.

Reference

1. B.E. Poling, J.M. Prausnitz, and J.P. O'Connell, *The Properties of Gases and Liquids*, 5th ed., McGraw Hill, 2000.

Application Library path: `Chemical_Reaction_Engineering_Module/Thermodynamics/droplet_evaporation_water_acetone`

Modeling Instructions

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

NEW

1. In the **New** window, Start by adding the individual physics interfaces for mass transfer, fluid flow, and heat transfer in fluids.
2. click **Model Wizard**.

MODEL WIZARD

1. In the **Model Wizard** window, click **2D Axisymmetric**.
2. In the **Select Physics** tree, select **Chemical Species Transport** > **Chemistry (chem)**.
3. Click **Add**.
4. In the **Select Physics** tree, select **Chemical Species Transport** > **Vapor–Liquid Equilibrium** > **Laminar Two-Phase Flow**.
5. Click **Add**.

6 In the **Added physics interfaces** tree, select **Transport of Concentrated Species in Vapor (tcs)**.

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

8 In the **Mass fractions (1)** table, enter the following settings:

wW
wN
wA

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

10 Click **Add**.

11 Click **Study**.

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

13 Click **Done**.

Add parameters by loading them from files. Optionally, enter parameters manually.

GLOBAL DEFINITIONS

Model Parameters

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 `droplet_evaporation_water_acetone_model_parameters.txt`.

5 In the **Label** text field, type `Model Parameters`.

Geometry Parameters

1 In the **Home** toolbar, click **Parameters** and choose **Add > Parameters**.

2 In the **Settings** window for **Parameters**, type `Geometry Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Add a **Thermodynamics** system that describes the thermodynamic properties in the model.

5 In the **Physics** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1 Go to the **Select System** window.

2 From the **Phase** list, choose **Vapor–liquid**.

3 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list box, select **acetone (67-64-1, C3H6O)**.

3 Click **+ Add Selected**.

4 In the **Species** list box, select **nitrogen (7727-37-9, N2)**.

5 Click **+ Add Selected**.

6 In the **Species** list box, select **water (7732-18-5, H2O)**.

7 Click **+ Add Selected**.

8 Click the **Next** button in the window toolbar.

SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.

2 From the list, choose **Ideal solution**.

3 From the **Gas-phase model** list, choose **Ideal gas**.

4 Click the **Finish** button in the window toolbar.

Continue by building the geometry for the system.

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 `Dc`.

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

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 `Dinj+Tw`.

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

5 Locate the **Position** section. In the **z** text field, type `Hc`.

Union 1 (uni1)

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

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

3 Click in the **Graphics** window and then press Ctrl+A to select both objects.

4 In the **Settings** window for **Union**, locate the **Union** section.

5 Clear the **Keep interior boundaries** checkbox.

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 `rd`.

4 In the **Sector angle** text field, type `90`.

Circle 2 (c2)

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 `2*rd`.

4 In the **Sector angle** text field, type `90`.

Union 2 (uni2)

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

2 Click in the **Graphics** window and then press Ctrl+A to select all objects.

Rectangle 3 (r3)

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 `Dc-Dinj-Tw`.

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

5 Locate the **Position** section. In the **r** text field, type `Dinj+Tw`.

6 In the **z** text field, type `Hc`.

Rectangle 4 (r4)

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 `Tw`.

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

5 Locate the **Position** section. In the **r** text field, type `Dinj`.

6 In the **z** text field, type `Hc`.

Union 3 (uni3)

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

2 Select the objects **r3** and **r4** only.

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

4 Clear the **Keep interior boundaries** checkbox.

Chamfer 1 (cha1)

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

2 On the object **uni3**, select Point 1 only.

3 In the **Settings** window for **Chamfer**, locate the **Distance** section.

4 In the **Distance from vertex** text field, type `0.75[mm]`.

Union 4 (uni4)

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

2 Click in the **Graphics** window and then press Ctrl+A to select both objects.

Rectangle 5 (r5)

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 `Dc`.

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

5 Locate the **Position** section. In the **z** text field, type `-Tw`.

6 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
`Layer 1`	`Dc-rd`

7 Select the **Layers to the right** checkbox.

8 Clear the **Layers on bottom** checkbox.

Form Union (fin)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Geometry 1** click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, locate the **Form Union/Assembly** section.

3 From the **Action** list, choose **Form an assembly**.

Ignore Edges 1 (ige1)

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

2 On the object **fin**, select Boundary 19 only.

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

There are boundaries in the geometry that were added to enable building a fine mesh around the droplet. Hiding these boundaries removes them from the graphics window, but they are still present, and available for meshing.

DEFINITIONS

Hide for Physics 1

1 In the **Model Builder** window, expand the **Definitions** node.

2 Right-click **View 1** and choose **Hide for Physics**.

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

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

5 Select Boundaries 4 and 25 only.

Add four materials. One material for the liquid phase, one for the vapor phase, one for the plastic channel roof, and one for the marble table.

GLOBAL DEFINITIONS

Vapor–Liquid System 1 (pp1)

In the **Model Builder** window, under **Global Definitions** > **Thermodynamics** right-click **Vapor–Liquid System 1 (pp1)** and choose **Generate Material**.

SELECT PHASE

1 Go to the **Select Phase** window.

2 From the list, choose **Liquid**.

3 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 Click **Remove All**.

3 In the list box, select **acetone**.

4 Click **Add Selected**.

5 In the list box, select **water**.

6 Click **Add Selected**.

7 Find the **Material composition** subsection. Click the **Mass fraction** button.

8 Click the **Next** button in the window toolbar.

SELECT PROPERTIES

1 Go to the **Select Properties** window.

2 Click the **Next** button in the window toolbar.

DEFINE MATERIAL

1 Go to the **Define Material** window.

2 Click the **Finish** button in the window toolbar.

GLOBAL DEFINITIONS

Inspect the material and add it to the proper selection.

MATERIALS

Liquid: acetone-water 1 (pp1mat1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** node, then click **Liquid: acetone-water 1 (pp1mat1)**.

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

3 Click **Clear Selection**.

4 Select Domain 3 only.

5 Locate the **Material Contents** section. Find the **Local properties** subsection. In the table, enter the following settings:

Name	Expression	Unit	Description	Property group
xw1	wA	1	Mass fraction, acetone	Basic
xw2	wW	1	Mass fraction, water	Basic

Add the vapor phase material. Use the nitrogen material already defined in a material library.

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 tree, select **Liquids and Gases** > **Gases** > **Nitrogen**.

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

MATERIALS

Nitrogen (mat1)

Select Domains 4 and 5 only.

The plastic material for the channel roof is available as a built in material.

ADD MATERIAL

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

2 In the tree, select **Built-in** > **Acrylic plastic**.

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

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

MATERIALS

Acrylic plastic (mat2)

Select Domain 6 only.

The marble material is available is the **Material Library**, included depending on license. For this example, define it manually.

Marble, Solid

1 In the **Model Builder** window, right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, type `Marble, Solid` in the **Label** text field.

3 Select Domains 1 and 2 only.

4 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** > **Marble, Solid (mat3)** node, then click **Basic (def)**.

5 In the **Settings** window for **Basic**, locate the **Output Properties** section.

6 Click **Select Quantity**.

7 In the **Physical Quantity** dialog, type `thermal` in the text field.

8 In the tree, select **Transport** > **Thermal conductivity (W/(m*K))**.

9 Click **OK**.

10 In the **Settings** window for **Basic**, locate the **Output Properties** section.

11 In the table, enter the following settings:

Property	Variable	Expression	Unit	Size
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	k_solid_average(T)	W/(m·K)	3x3

12 Click **Select Quantity**.

13 In the **Physical Quantity** dialog, select **General** > **Density (kg/m^3)** in the tree.

14 Click **OK**.

15 In the **Settings** window for **Basic**, locate the **Output Properties** section.

16 In the table, enter the following settings:

Property	Variable	Expression	Unit	Size
Density	rho	rho_marble	kg/m³	1x1

17 Click **Select Quantity**.

18 In the **Physical Quantity** dialog, type heat in the text field.

19 In the tree, select **Transport** > **Heat capacity at constant pressure (J/(kg*K))**.

20 Click **OK**.

21 In the **Settings** window for **Basic**, locate the **Output Properties** section.

22 In the table, enter the following settings:

Property	Variable	Expression	Unit	Size
Heat capacity at constant pressure	Cp	cp_marble	J/(kg·K)	1x1

Piecewise 1 (pw1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global** > **Piecewise**.

2 In the **Settings** window for **Piecewise**, type k_solid_average in the **Function name** text field.

3 Locate the **Definition** section. In the **Argument** text field, type T.

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

Start	End	Function
273	473	9.04871122-0.0392846005*T^1+7.8563479E-5*T^2-5.57866051E-8*T^3

5 Locate the **Units** section. In the **Arguments** text field, type K.

6 In the **Function** text field, type `W/m/K`.

Add selections to the **Deforming Domain** and **Symmetry Roller** subfeatures in the **Moving Mesh** feature. This is needed to model the shrinkage of the droplet as a result of the evaporation.

MOVING MESH

Deforming Domain 1

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

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

3 Click **Clear Selection**.

4 Select Domains 3 and 4 only.

Symmetry/Roller 1

1 In the **Moving Mesh** toolbar, click **Symmetry/Roller**.

2 Select Boundaries 8–10 and 17 only.

Before setting up the physics of the system, add some selections. These are useful when setting up the physics.

DEFINITIONS

Vapor

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 4 and 5 only.

Liquid

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domain 3 only.

Walls

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 1, 2, and 6 only.

Inflow

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 13 only.

5 In the **Label** text field, type `Inflow`.

Outflow

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 22 only.

Vapor-Liquid Interface

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, type `Vapor-Liquid Interface` in the **Label** text field.

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 24 only.

Fluids

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Fluids` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **Vapor** and **Liquid**.

5 Click **OK**.

Now, define the chemistry and physics of the model. Begin by adding chemical species to the **Chemistry** interface. Then connect this interface, and the **Transport of Concentrated Species in Vapor** interface to **Thermodynamics**.

CHEMISTRY (CHEM)

Species 1

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

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

3 In the text field, type `Water`.

4 Locate the **Chemical Formula** section. Select the **Enable formula** checkbox.

5 In the text field, type `H2O`.

6 In the **Physics** toolbar, click **Domains** and choose **Species**.

1 In the **Settings** window for **Species**, locate the **Name** section.

2 In the text field, type `Acetone`.

3 Locate the **Chemical Formula** section. Select the **Enable formula** checkbox.

4 In the text field, type `C3H6O`.

5 In the **Physics** toolbar, click **Domains** and choose **Species**.

1 In the **Settings** window for **Species**, locate the **Name** section.

2 In the text field, type `N2`.

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

4 In the **Settings** window for **Chemistry**, locate the **Mixture Properties** section.

5 From the **Type** list, choose **Concentrated species**.

6 Select the **Thermodynamics** checkbox.

7 Locate the **Species Matching** section. Find the **Bulk species** subsection. In the table, enter the following settings:

Species	**Type**	**Mass fraction**	**Value (1)**	**From Thermodynamics**
Acetone	Free species	User defined	1	C3H6O
N2	Free species	User defined	1	N2
Water	Free species	User defined	1	H2O

8 From the **Species solved for** list, choose **Transport of Concentrated Species in Vapor**.

9 In the table, enter the following settings:

Species	**Type**	**Mass fraction**	**Value (1)**	**From Thermodynamics**
Acetone	Free species	wA	Solved for	C3H6O
N2	Free species	wN	Solved for	N2
Water	Free species	wW	Solved for	H2O

Define the mass transfer in the system.

TRANSPORT OF CONCENTRATED SPECIES IN VAPOR (TCS)

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

2 In the **Settings** window for **Transport of Concentrated Species in Vapor**, locate the **Domain Selection** section.

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

4 Locate the **Species** section. From the **From mass constraint** list, choose **wN**.

Fluid - Vapor

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

2 In the **Settings** window for **Fluid**, type `Fluid - Vapor` in the **Label** text field.

3 Locate the **Model Input** section. Click **Make All Model Inputs Editable** in the upper-right corner of the section.

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

5 From the T list, choose **Temperature (nirf1)**.

Fluid - Liquid

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

2 In the **Settings** window for **Fluid**, type `Fluid - Liquid` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Liquid**.

4 Locate the **Density** section. From the ρ list, choose **User defined**. In the associated text field, type `pp1mat1.def.rho`.

5 Locate the **Diffusion** section. In the table, enter the following settings:

Species 1	**Species 2**	**Diffusivity**	**Diffusion coefficient (m^2/s)**
wW	wN	User defined	`1e-9[m^2/s]`
wW	wA	User defined	`1e-9[m^2/s]`
wN	wA	User defined	`1e-9[m^2/s]`

Add the initial mass fractions in the system. The vapor phase consists of pure nitrogen, while the drop consists of only water and acetone. For numerical reasons, the mass fraction of nitrogen in the drop cannot be zero, and is therefor set to a very low value.

Initial Values - Vapor

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 $\omega_{0,\mathrm{wW}}$ text field, type `0`.

4 In the $\omega_{0,\mathrm{wA}}$ text field, type `0`.

5 In the **Label** text field, type `Initial Values - Vapor`.

Initial Values - Liquid

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

2 In the **Settings** window for **Initial Values**, type `Initial Values - Liquid` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Liquid**.

4 Locate the **Initial Values** section. In the $\omega_{0,\mathrm{wW}}$ text field, type `0.799`.

5 In the $\omega_{0,\mathrm{wA}}$ text field, type `0.2009`.

Specify the inlet conditions in the **Vapor Inflow** feature.

Vapor Inflow 1

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

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

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

4 Locate the **Vapor Inflow** section. Select the **Relative humidity** checkbox.

5 In the ϕ_{w} text field, type `0.3`.

6 Find the **Upstream properties** subsection. In the T_{Vap} text field, type `T0`.

7 Locate the **Transient Initialization** section. Select the **Enable** checkbox.

8 From the **Duration** list, choose **User defined**. In the Δt text field, type `1`.

Add an **Outflow** boundary condition.

Outflow 1

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

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

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

Vapor–Liquid-Solution Interface 1

1 In the **Model Builder** window, click **Vapor–Liquid-Solution Interface 1**.

2 In the **Settings** window for **Vapor–Liquid-Solution Interface**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Vapor-Liquid Interface**.

4 Locate the **Vapor Equilibrium** section. From the **Liquid** list, choose **Thermochemistry coupling**.

5 From the **Chemistry** list, choose **Chemistry (chem)**.

6 Find the **Evaporating/condensing species** subsection. Select the **wW, H2O (water)** checkbox.

7 Select the **wA, C3H6O (acetone)** checkbox.

8 Locate the **Liquid Side** section. Select the **Reverse direction** checkbox.

9 Locate the **Transient Initialization** section. From the **Duration** list, choose **User defined**. In the Δt text field, type `1`.

10 Click to expand the **Constraint Settings** section.

The **Vapor–Liquid Interface** node is for interfaces where the liquid side composition is assumed constant. It is not used in this model and can be deleted.

Vapor–Liquid Interface 1

In the **Model Builder** window, right-click **Vapor–Liquid Interface 1** and choose **Delete**.

The mass transfer part of the system has been defined. Now, define the fluid flow in the system.

LAMINAR FLOW (SPF)

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

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

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

4 Locate the **Physical Model** section. Select the **Include gravity** checkbox.

5 In the p_{ref} text field, type `p0`.

Fluid Properties - Vapor

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

2 In the **Settings** window for **Fluid Properties**, type `Fluid Properties - Vapor` in the **Label** text field.

Add a **Step** function that can be used to initialize the study.

DEFINITIONS

Step 1 (step1)

1 In the **Definitions** toolbar, click f(x) **More Functions** and choose **Step**.

2 In the **Settings** window for **Step**, type `gStep` in the **Function name** text field.

3 Locate the **Parameters** section. In the **Location** text field, type `0.5*tgInit`.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type `tgInit`.

LAMINAR FLOW (SPF)

Initial Values 1

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

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

3 Clear the **Compensate for hydrostatic pressure approximation** checkbox.

Gravity 1

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

2 In the **Settings** window for **Gravity**, locate the **Acceleration of Gravity** section.

3 Specify the **g** vector as

-g_const*(gStep(t)*init+(1-init))	z

Wall 2

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

2 Select Boundaries 9 and 17 only.

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

4 From the **Wall condition** list, choose **Navier slip**.

Fluid Properties - Liquid

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

2 In the **Settings** window for **Fluid Properties**, type `Fluid Properties - Liquid` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Liquid**.

4 Locate the **Model Input** section. Click **Make All Model Inputs Editable** in the upper-right corner of the section.

5 In the p_A text field, type `p0`.

Fluid-Fluid Interface 1

1 In the **Model Builder** window, click **Fluid-Fluid Interface 1**.

2 In the **Settings** window for **Fluid-Fluid Interface**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Vapor-Liquid Interface**.

4 Locate the **Normal Direction** section. Select the **Reverse normal direction** checkbox.

5 Locate the **Mass Flux** section. From the M_f list, choose **Total evaporative mass flux (tcs/vlm1)**.

Contact Angle 1

1 In the **Model Builder** window, expand the **Fluid-Fluid Interface 1** node, then click **Contact Angle 1**.

2 In the **Settings** window for **Contact Angle**, locate the **Contact Angle** section.

3 In the θ_w text field, type `theta`.

Inlet 1

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

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

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

4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `Uin*(gStep(t)*init+(1-init))`.

Outlet 1

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

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

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

4 Locate the **Pressure Conditions** section. Select the **Normal flow** checkbox.

Continue by defining the heat transfer in the system.

HEAT TRANSFER IN FLUIDS (HT)

Fluid - Vapor

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

2 In the **Settings** window for **Fluid**, type `Fluid - Vapor` in the **Label** text field.

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 `T0`.

Fluid - Liquid

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

2 In the **Settings** window for **Fluid**, type `Fluid - Liquid` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Liquid**.

4 Locate the **Model Input** section. Click **Make All Model Inputs Editable** in the upper-right corner of the section.

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

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

7 Locate the **Heat Convection** section. From the **u** list, choose **Velocity field (spf)**.

Solid 1

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

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

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

Boundary Heat Source 1

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

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

3 From the **Selection** list, choose **Vapor-Liquid Interface**.

4 Locate the **Boundary Heat Source** section. From the Q_{b} list, choose **Heat of evaporation (tcs/vlm1)**.

Inflow 1

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

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

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

4 Locate the **Upstream Properties** section. In the T_{ustr} text field, type `T0`.

Temperature 1

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

2 Select Boundaries 2, 5, 19, and 20 only.

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

4 In the T_0 text field, type `T0`.

Set up the mesh.

MESH 1

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

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

3 From the list, choose **User-controlled mesh**.

Size

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

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

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

Size 1

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

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

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

4 Locate the **Element Size** section. From the **Predefined** list, choose **Fine**.

Size 2

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

2 Select Boundaries 14, 17, 18, and 21 only.

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

4 From the **Predefined** list, choose **Extra fine**.

Edge 1

1 In the **Mesh** toolbar, click **More Generators** and choose **Edge**.

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

3 From the **Selection** list, choose **Vapor-Liquid Interface**.

Distribution 1

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

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

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type 100.

5 In the **Element ratio** text field, type 2.

Free Triangular 1

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

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

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

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

Size: Evaporation Zone

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, type `Size: Evaporation Zone` in the **Label** text field.

3 Select Domain 4 only.

4 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

5 Click the **Custom** button.

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

7 Select the **Maximum element size** checkbox. In the associated text field, type `2.6E-4`.

8 Select the **Maximum element growth rate** checkbox. In the associated text field, type `1.05`.

Size: Interface

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, type `Size: Interface` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Vapor-Liquid Interface**.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 Click the **Custom** button.

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

8 Select the **Maximum element size** checkbox. In the associated text field, type `1E-4`.

Size: Droplet Top

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, type `Size: Droplet Top` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Point**.

4 Select Point 8 only.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 Click the **Custom** button.

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

8 Select the **Maximum element size** checkbox. In the associated text field, type `0.1E-4`.

Size: Droplet Edge

1 Right-click **Free Triangular 1** and choose **Size**.

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

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

4 Select Point 14 only.

5 In the **Label** text field, type `Size: Droplet Edge`.

6 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

7 Click the **Custom** button.

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

9 Select the **Maximum element size** checkbox. In the associated text field, type `0.5E-4`.

Size: Droplet

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, type `Size: Droplet` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Liquid**.

4 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

5 Click the **Custom** button.

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

7 Select the **Maximum element size** checkbox. In the associated text field, type `1E-4`.

Size: Droplet Center

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, type `Size: Droplet Center` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Point**.

4 Select Point 7 only.

5 Locate the **Element Size** section. Click the **Custom** button.

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

7 Select the **Maximum element size** checkbox. In the associated text field, type `0.5e-4`.

Free Triangular 2

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

2 Drag and drop below **Free Triangular 1**.

Size 1

1 Right-click **Free Triangular 2** and choose **Size**.

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

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

4 Select Boundary 3 only.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 Click the **Custom** button.

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

8 Select the **Maximum element size** checkbox. In the associated text field, type `1E-4`.

Size 2

1 In the **Model Builder** window, right-click **Free Triangular 2** and choose **Size**.

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

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

4 Select Point 7 only.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

6 Click the **Custom** button.

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

8 Select the **Maximum element size** checkbox. In the associated text field, type `0.25E-4`.

Boundary Layers 1

1 In the **Mesh** toolbar, click **Boundary Layers**.

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

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

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

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 14, 15, 17, 18, and 21 only.

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

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

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

Boundary Layer Properties 1

1 In the **Mesh** toolbar, click **More Attributes** and choose **Boundary Layer Properties**.

2 Select Boundaries 8, 9, and 24 only.

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

4 In the **Number of layers** text field, type `6`.

5 In the **Thickness adjustment factor** text field, type `2.5`.

Boundary Layers 2

1 In the **Mesh** toolbar, click **Boundary Layers**.

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

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

4 Select Domains 1 and 2 only.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 3 and 6 only.

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

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

5 In the **Thickness adjustment factor** text field, type `3`.

Edge 1

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

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

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

Set up the study.

STUDY 1: DROPLET INITIALIZATION

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

2 In the **Settings** window for **Study**, type `Study 1: Droplet Initialization` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1: Droplet Initialization** click **Step 1: Time Dependent**.

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

3 In the **Output times** text field, type `range(0,0.05,1)*tgInit range(2,1,5)`.

4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Transport of Concentrated Species in Vapor (tcs)** and **Heat Transfer in Fluids (ht)**.

5 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

6 Click **Add**.

7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
init (Initialization step)	1	

Edit the default scale for the velocity to improve the convergence rate.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 1**.

3 In the **Settings** window for **Dependent Variables**, locate the **Residual Scaling** section.

4 From the **Method** list, choose **Manual**.

5 In the **Model Builder** window, expand the **Study 1: Droplet Initialization** > **Solver Configurations** > **Solution 1 (sol1)** > **Dependent Variables 1** node, then click **Velocity Field (Spatial Frame) (comp1.u)**.

6 In the **Settings** window for **Field**, locate the **Scaling** section.

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

8 Click in the **Scale** text field, then press Ctrl+Space. From the menu, choose **Uin - Inlet velocity - m/s**.

Now compute the study.

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

RESULTS

Velocity (spf)

Inspect the resulting default plots, then add a second study that solves for not only the fluid dynamics, but also the mass and heat transfer. Use the results from the first study as a starting point.

ADD STUDY

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

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

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

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

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

STUDY 2

Step 1: Time Dependent

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

2 In the **Output times** text field, type `0 1200`.

3 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1: Droplet Initialization, Time Dependent**.

6 From the **Selection** list, choose **Last**.

Rename the study. Also apply an initial time step, define manual scales, and change the Jacobian update strategy.

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

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

Solution 2 (sol2)

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

Use an initial time step that is short compared to the 1 s of initialization used for the vapor–liquid equilibrium.

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

4 From the **Times to store** list, choose **Steps taken by solver**.

5 In the **Store every Nth step** text field, type `2`.

6 Click to expand the **Time Stepping** section.

7 Select the **Initial step** checkbox. In the associated text field, type `0.01`.

A recommended modeling practice for time-dependent models is to define manual scales. This allows the solver to time step efficiently while maintaining the required accuracy. Here the velocity and pressure scales are taken from the previous study and the initial temperature is used. For the mass fractions the scales are set to 0.01.

8 In the **Model Builder** window, expand the **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** node, then click **Pressure (comp1.p)**.

9 In the **Settings** window for **Field**, locate the **Scaling** section.

10 From the **Method** list, choose **Initial-value based**.

11 In the **Model Builder** window, under **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** click **Temperature (comp1.T)**.

12 In the **Settings** window for **Field**, locate the **Scaling** section.

13 From the **Method** list, choose **Manual**.

14 In the **Scale** text field, type `T0`.

15 In the **Model Builder** window, under **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** click **Velocity Field (Spatial Frame) (comp1.u)**.

16 In the **Settings** window for **Field**, locate the **Scaling** section.

17 From the **Method** list, choose **Initial-value based**.

18 In the **Model Builder** window, under **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** click **Mass Fraction (comp1.wA)**.

19 In the **Settings** window for **Field**, locate the **Scaling** section.

20 From the **Method** list, choose **Manual**.

21 In the **Scale** text field, type `0.01`.

22 In the **Model Builder** window, under **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Dependent Variables 1** click **Mass Fraction (comp1.wW)**.

23 In the **Settings** window for **Field**, locate the **Scaling** section.

24 From the **Method** list, choose **Manual**.

25 In the **Scale** text field, type `0.01`.

26 In the **Model Builder** window, expand the **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Time-Dependent Solver 1** node.

The current model includes a number of nonlinear couplings across the vapor–liquid interface. Change to update the Jacobian in every iteration for a more robust simulation. This is more time consuming, but on the other hand a higher damping factor can be used.

27 In the **Model Builder** window, expand the **Study 2: Evaporation** > **Solver Configurations** > **Solution 2 (sol2)** > **Time-Dependent Solver 1** > **Segregated 1** node, then click **Reacting Flow**.

28 In the **Settings** window for **Segregated Step**, click to expand the **Method and Termination** section.

29 From the **Jacobian update** list, choose **On every iteration**.

30 In the **Damping factor** text field, type `0.8`.

Compute the study.

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

RESULTS

Vapor Pressure, W (tcs)

Add the result nodes from the first study to a group.

Moving Mesh, Pressure (spf), Velocity (spf), Velocity, 3D (spf)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Velocity (spf)**, **Pressure (spf)**, **Velocity, 3D (spf)**, and **Moving Mesh**.

2 Right-click and choose **Group**.

Droplet Initialization

In the **Settings** window for **Group**, type `Droplet Initialization` in the **Label** text field.

Inspect the default plots, then modify them to your preferences. Start by adding custom datasets.

Study 2: Evaporation: All Phases

1 In the **Model Builder** window, expand the **Results** > **Datasets** node, then click **Study 2: Evaporation/Solution 2 (sol2)**.

2 In the **Settings** window for **Solution**, type `Study 2: Evaporation: All Phases` in the **Label** text field.

Study 2: Evaporation: Vapor

1 Right-click **Study 2: Evaporation: All Phases** and choose **Duplicate**.

2 In the **Settings** window for **Solution**, type `Study 2: Evaporation: Vapor` in the **Label** text field.

Selection

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

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

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

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

Study 2: Evaporation: Liquid

1 In the **Model Builder** window, under **Results** > **Datasets** right-click **Study 2: Evaporation: Vapor (sol2)** and choose **Duplicate**.

2 In the **Model Builder** window, click **Study 2: Evaporation: Vapor 1 (sol2)**.

3 In the **Settings** window for **Solution**, type `Study 2: Evaporation: Liquid` in the **Label** text field.

Selection

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

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

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

Study 2: Evaporation: Table

1 In the **Model Builder** window, under **Results** > **Datasets** right-click **Study 2: Evaporation: Liquid (sol2)** and choose **Duplicate**.

2 In the **Model Builder** window, click **Study 2: Evaporation: Liquid 1 (sol2)**.

3 In the **Settings** window for **Solution**, type `Study 2: Evaporation: Table` in the **Label** text field.

Selection

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

2 Select Domains 1 and 2 only.

Use these datasets to create **Revolution** datasets.

Revolution 2D 4

In the **Model Builder** window, under **Results** > **Datasets** right-click **Revolution 2D 2** and choose **Duplicate**.

Revolution: Vapor

1 In the **Settings** window for **Revolution 2D**, type `Revolution: Vapor` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Evaporation: Vapor (sol2)**.

Revolution: Vapor 1

Right-click **Revolution: Vapor** and choose **Duplicate**.

Revolution: Liquid

1 In the **Settings** window for **Revolution 2D**, type `Revolution: Liquid` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Evaporation: Liquid (sol2)**.

Revolution: Liquid 1

Right-click **Revolution: Liquid** and choose **Duplicate**.

Revolution: Table

1 In the **Settings** window for **Revolution 2D**, type `Revolution: Table` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Evaporation: Table (sol2)**.

Finally, add a **Cut Plane** and a **Mirror** dataset.

Cut Plane: Vapor

1 In the **Results** toolbar, click **Cut Plane**.

2 In the **Settings** window for **Cut Plane**, type `Cut Plane: Vapor` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Revolution: Vapor**.

Mirror 2D 1

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

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

3 From the **Dataset** list, choose **Study 2: Evaporation: All Phases (sol2)**.

Set up a plot of the fluid velocity in the system. Use the default plot as the starting point.

Vapor and Liquid Flow

1 In the **Model Builder** window, under **Results** click **Velocity (spf) 1**.

2 In the **Settings** window for **2D Plot Group**, type `Vapor and Liquid Flow` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

5 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.

6 Select the **Show titles** checkbox.

7 Select the **Show units** checkbox.

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

Velocity in Vapor

1 In the **Model Builder** window, expand the **Vapor and Liquid Flow** node, then click **Surface**.
2 In the **Settings** window for **Surface**, type `Velocity in Vapor` in the **Label** text field.
3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Pelagic**.
4 In the **Color legend title** text field, type `Vapor`.

Selection 1

1 Right-click **Velocity in Vapor** and choose **Selection**.
2 In the **Settings** window for **Selection**, locate the **Selection** section.
3 From the **Selection** list, choose **Vapor**.

Velocity in Liquid

1 Right-click **Velocity in Vapor** and choose **Duplicate**.
2 In the **Settings** window for **Surface**, type `Velocity in Liquid` in the **Label** text field.
3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Acanthaster**.
4 In the **Color legend title** text field, type `Liquid`.

Selection 1

1 In the **Model Builder** window, expand the **Velocity in Liquid** node, then click **Selection 1**.
2 In the **Settings** window for **Selection**, locate the **Selection** section.
3 From the **Selection** list, choose **Liquid**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Vapor and Liquid Flow** and choose **Arrow Surface**.
2 In the **Settings** window for **Arrow Surface**, locate the **Expression** section.
3 In the **r-component** text field, type `u`.
4 In the **z-component** text field, type `w`.
5 Locate the **Arrow Positioning** section. Find the **r grid points** subsection. In the **Points** text field, type `40`.
6 Locate the **Coloring and Style** section. From the **Arrow length** list, choose **Logarithmic**.
7 From the **Color** list, choose **Custom**.
8 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.
9 Click **Define custom colors**.
10 Set the RGB values to 11, 86, and 143, respectively.

11 Click **Add to custom colors**.

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

Selection 1

1 Right-click **Arrow Surface 1** and choose **Selection**.
2 In the **Settings** window for **Selection**, locate the **Selection** section.
3 From the **Selection** list, choose **Vapor**.

Arrow Surface 2

1 In the **Model Builder** window, under **Results** > **Vapor and Liquid Flow** right-click **Arrow Surface 1** and choose **Duplicate**.
2 In the **Settings** window for **Arrow Surface**, locate the **Arrow Positioning** section.
3 Find the **r grid points** subsection. In the **Points** text field, type `12`.
4 Find the **z grid points** subsection. In the **Points** text field, type `12`.
5 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

Selection 1

1 In the **Model Builder** window, expand the **Arrow Surface 2** node, then click **Selection 1**.
2 In the **Settings** window for **Selection**, locate the **Selection** section.
3 From the **Selection** list, choose **Liquid**.
4 In the **Vapor and Liquid Flow** toolbar, click **Plot**.

Vapor and Liquid Flow

Use a dedicated view to visualize the droplet without the need to zoom repeatedly.

1 In the **Model Builder** window, under **Results** click **Vapor and Liquid Flow**.
2 In the **Settings** window for **2D Plot Group**, locate the **Plot Settings** section.
3 From the **View** list, choose **New view**.
4 In the **Vapor and Liquid Flow** toolbar, click **Plot** to create the view. Now give it a suitable name.
5 Click **Go to Source**.

View Flow

1 In the **Model Builder** window, under **Results** > **Views** click **View 2D 2**.
2 In the **Settings** window for **View 2D**, type `View Flow` in the **Label** text field.

Modify the camera according to your preferences. An example of settings for the added view can be seen by opening the Application Library model.

Vapor and Liquid Flow

Edit the time to see the shrinkage of the drop.

1 In the **Model Builder** window, under **Results** click **Vapor and Liquid Flow**.
2 In the **Settings** window for **2D Plot Group**, click **Plot First**.
3 Click **Plot Next**.

Create a plot that illustrates the mass fraction and partial pressure of acetone in the system.

Acetone

1 In the **Model Builder** window, under **Results** click **Vapor Pressure, A (tcs)**.
2 In the **Settings** window for **2D Plot Group**, type `Acetone` in the **Label** text field.
3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 2D 1**.
4 From the **Time (s)** list, choose **Interpolation**.
5 In the **Time** text field, type `60`.
6 Locate the **Title** section. From the **Title type** list, choose **None**.
7 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
8 Select the **Show units** checkbox.
9 From the **Position** list, choose **Right double**.

Vapor Pressure

1 In the **Model Builder** window, expand the **Acetone** node, then click **Surface 1**.
2 In the **Settings** window for **Surface**, type `Vapor Pressure` in the **Label** text field.
3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Amethyst**.

Selection 1

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

Liquid Concentration

1 Right-click **Vapor Pressure** and choose **Duplicate**.
2 In the **Settings** window for **Surface**, type `Liquid Concentration` in the **Label** text field.
3 Locate the **Expression** section. In the **Expression** text field, type `tcs.c_wA`.
4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Arctium**.

Selection 1

1 In the **Model Builder** window, expand the **Liquid Concentration** node, then click **Selection 1**.

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

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

Arrow Surface 1

In the **Model Builder** window, under **Results** > **Acetone** right-click **Arrow Surface 1** and choose **Delete**.

Streamline 1

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

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

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

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

5 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.

6 In the **Density level** text field, type `7.8`.

7 From the **Advanced parameters** list, choose **Manual**.

8 In the **Terminating distance factor** text field, type `0.1`.

9 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

10 Select the **Number of arrows** checkbox. In the associated text field, type `300`.

11 Select the **Scale factor** checkbox. In the associated text field, type `0.002`.

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

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

14 Click **Define custom colors**.

15 Set the RGB values to 0, 85, and 150, respectively.

16 Click **Add to custom colors**.

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

Selection 1

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

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

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

Add a **View**, and hide the dataset edges.

View Mirror

1 In the **Model Builder** window, under **Results** right-click **Views** and choose **View 2D**.

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

Acetone

1 In the **Model Builder** window, expand the **View Mirror** node, then click **Results** > **Acetone**.

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

3 From the **View** list, choose **View Mirror**.

4 Clear the **Plot dataset edges** checkbox.

5 In the **Acetone** toolbar, click **Plot**.

Add a plot of the temperature in the drop.

Temperature

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

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

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

Temperature

1 In the **Model Builder** window, under **Results** > **Temperature** click **Vapor Pressure**.

2 In the **Settings** window for **Surface**, type `Temperature` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `T`.

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

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

Liquid Concentration

In the **Model Builder** window, right-click **Liquid Concentration** and choose **Delete**.

Selection 1

1 In the **Model Builder** window, expand the **Results** > **Temperature** > **Temperature** node, then click **Selection 1**.

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

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

Line 1

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

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

3 In the **Expression** text field, type `1`.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Black**.

Selection 1

1 Right-click **Line 1** and choose **Selection**.

2 Select Boundaries 2, 5, 19, and 20 only.

Temperature

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

2 In the **Temperature** toolbar, click **Plot**.

Add a plot of the density in the system.

Density

1 In the **Model Builder** window, right-click **Acetone** and choose **Duplicate**.

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

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

Vapor Density

1 In the **Model Builder** window, under **Results** > **Density** click **Vapor Pressure**.

2 In the **Settings** window for **Surface**, type `Vapor Density` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `tcs.rho`.

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

Liquid Density

1 In the **Model Builder** window, under **Results** > **Density** click **Liquid Concentration**.

2 In the **Settings** window for **Surface**, type `Liquid Density` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `tcs.rho`.

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

5 In the **Density** toolbar, click **Plot**.

Make a plot showing the water partial pressure and the water concentration in the drop.

Water

1 In the **Model Builder** window, right-click **Acetone** and choose **Duplicate**.

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

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

Vapor Pressure

1 In the **Model Builder** window, click **Vapor Pressure**.

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

3 In the **Expression** text field, type `tcs.p_wW`.

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

Liquid Concentration

1 In the **Model Builder** window, click **Liquid Concentration**.

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

3 In the **Expression** text field, type `tcs.c_wW`.

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

5 In the **Water** toolbar, click **Plot**.

Make an animation to see the changes without the need to change the time manually.

Water

In the **Model Builder** window, click **Water**.

Animation 1

1 In the **Water** toolbar, click **Animation** and choose **Player**.

2 In the **Settings** window for **Animation**, click **Show Frame**.

3 Click the **Play** button in the **Graphics** toolbar.

Set up some line graphs that illustrate the evaporation rate, the droplet temperature, the shrinkage, and the top position of the drop. Add an **Evaluation Group** to derive the evaporation rate.

Evaluation Group: Evaporation Rate

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group: Evaporation Rate` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Evaporation: All Phases (sol2)**.

Line Integration 1

1 Right-click **Evaluation Group: Evaporation Rate** and choose **Integration** > **Line Integration**.

2 Select Boundary 24 only.

3 In the **Settings** window for **Line Integration**, locate the **Expressions** section.

4 In the table, enter the following settings:

Expression	**Unit**	**Description**
abs(tcs.jV_wA)	kg/s	Evaporative mass flux, Acetone

Line Integration 2

1 Right-click **Line Integration 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	**Unit**	**Description**
abs(tcs.jV_wW)	kg/s	Evaporative mass flux, Water

Line Integration 3

1 Right-click **Line Integration 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	**Unit**	**Description**
abs(tcs.jV)	kg/s	Evaporative mass flux, Total

Evaluate the integrals and plot the data using a **Table Graph**.

4 In the **Evaluation Group: Evaporation Rate** toolbar, click **Evaluate**.

EVALUATION GROUP: EVAPORATION RATE

1 Go to the **Evaluation Group: Evaporation Rate** window.

2 Click the **Table Graph** button in the window toolbar.

RESULTS

Table Graph 1

1 In the **Settings** window for **Table Graph**, click to expand the **Legends** section.

2 Select the **Show legends** checkbox.

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

4 In the table, enter the following settings:

Legends
`Acetone (kg/s)`
`Water (kg/s)`
`Total (kg/s)`

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

Evaporation Rate

1 In the **Model Builder** window, under **Results** click **1D Plot Group 19**.

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

3 In the **Evaporation Rate** toolbar, click **Plot**.

Plot the temperature in the drop.

Evaluation Group: Droplet Temperature

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type `Evaluation Group: Droplet Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Evaporation: All Phases (sol2)**.

T, Top

1 Right-click **Evaluation Group: Droplet Temperature** and choose **Point Evaluation**.

2 In the **Settings** window for **Point Evaluation**, type `T, Top` in the **Label** text field.

3 Select Point 8 only.

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

Expression	Unit	Description
`T`	`K`	`T, top`

T, Contact

1 In the **Model Builder** window, right-click **Evaluation Group: Droplet Temperature** and choose **Point Evaluation**.

2 In the **Settings** window for **Point Evaluation**, type `T, Contact` in the **Label** text field.

3 Select Point 14 only.

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

Expression	Unit	Description
T	K	T, contact

Evaluation Group: Droplet Temperature

1 In the **Model Builder** window, click **Evaluation Group: Droplet Temperature**.

2 In the **Evaluation Group: Droplet Temperature** toolbar, click **Evaluate**.

EVALUATION GROUP: DROPLET TEMPERATURE

1 Go to the **Evaluation Group: Droplet Temperature** window.

2 Click the **Table Graph** button in the window toolbar.

RESULTS

Table Graph 1

1 In the **Settings** window for **Table Graph**, locate the **Legends** section.

2 Select the **Show legends** checkbox.

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

4 In the table, enter the following settings:

Legends
T, top (K)
T, contact (K)

5 In the **1D Plot Group 20** toolbar, click **Plot**.

Droplet Temperature

1 In the **Model Builder** window, under **Results** click **1D Plot Group 20**.

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

Add a graph that illustrates the droplet shrinkage.

Evaluation Group: Droplet Shrinkage

1 In the **Model Builder** window, right-click **Evaluation Group: Droplet Temperature** and choose **Duplicate**.

2 In the **Model Builder** window, click **Evaluation Group: Droplet Temperature 1**.

3 In the **Settings** window for **Evaluation Group**, type `Evaluation Group: Droplet Shrinkage` in the **Label** text field.

rd, Top

1 In the **Model Builder** window, under **Results** > **Evaluation Group: Droplet Shrinkage** click **T, Top**.
2 In the **Settings** window for **Point Evaluation**, type `rd, Top` in the **Label** text field.
3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
z	m	rd, top

4 Locate the **Data Series Operation** section. From the **Normalization** list, choose **First**.

rd, Contact

1 In the **Model Builder** window, under **Results** > **Evaluation Group: Droplet Shrinkage** click **T, Contact**.
2 In the **Settings** window for **Point Evaluation**, type `rd, Contact` in the **Label** text field.
3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
r	m	rd, contact

4 Locate the **Data Series Operation** section. From the **Normalization** list, choose **First**.

Surface Integration 1

1 In the **Model Builder** window, right-click **Evaluation Group: Droplet Shrinkage** and choose **Integration** > **Surface Integration**.
2 Select Domain 3 only.
3 In the **Settings** window for **Surface Integration**, locate the **Expressions** section.
4 In the table, enter the following settings:

Expression	Unit	Description
1	m^3	

5 Locate the **Data Series Operation** section. From the **Normalization** list, choose **First**.

Evaluation Group: Droplet Shrinkage

1 In the **Model Builder** window, click **Evaluation Group: Droplet Shrinkage**.
2 In the **Evaluation Group: Droplet Shrinkage** toolbar, click **Evaluate**.

EVALUATION GROUP: DROPLET SHRINKAGE

1 Go to the **Evaluation Group: Droplet Shrinkage** window.

2 Click the **Table Graph** button in the window toolbar.

RESULTS

Table Graph 1

1 In the **Settings** window for **Table Graph**, locate the **Legends** section.

2 Select the **Show legends** checkbox.

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

4 In the table, enter the following settings:

Legends
`Top position`
`Contact point`
`Volume`

Droplet Shrinkage

1 In the **Model Builder** window, under **Results** click **1D Plot Group 21**.

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

3 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

4 In the **Droplet Shrinkage** toolbar, click **Plot**.

The steps below describes how to set up the plot **Acetone Mass Fraction and Partial Pressure**.

Acetone Mass Fraction and Partial Pressure

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Acetone Mass Fraction and Partial Pressure` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Revolution: Liquid**.

4 From the **Time (s)** list, choose **Interpolation**.

5 In the **Time** text field, type `300`.

6 Click to expand the **Title** section. From the **Title type** list, choose **None**.

7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

Isosurface 1

1 Right-click **Acetone Mass Fraction and Partial Pressure** and choose **Isosurface**.

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

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

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

5 Locate the **Levels** section. In the **Total levels** text field, type 9.

Acetone Mass Fraction and Partial Pressure

1 In the **Model Builder** window, click **Acetone Mass Fraction and Partial Pressure**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 From the **View** list, choose **View 3D 5**.

Surface 1

1 Right-click **Acetone Mass Fraction and Partial Pressure** and choose **Surface**.

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

3 From the **Dataset** list, choose **Revolution: Table**.

4 Locate the **Expression** section. In the **Expression** text field, type T.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Kyanite**.

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

Material Appearance 1

1 Right-click **Surface 1** and choose **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

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

5 Locate the **Color** section. Select the **Use the plot's color** checkbox.

Acetone Mass Fraction and Partial Pressure

1 In the **Model Builder** window, under **Results** click **Acetone Mass Fraction and Partial Pressure**.

2 In the **Settings** window for **3D Plot Group**, locate the **Color Legend** section.

3 Select the **Show units** checkbox.

Streamline Surface 1

1 In the **Acetone Mass Fraction and Partial Pressure** toolbar, click **More Plots** and choose **Streamline Surface**.

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

3 From the **Dataset** list, choose **Cut Plane: Vapor**.

4 From the **Solution parameters** list, choose **From parent**.

5 Locate the **Expression** section. In the **x-component** text field, type `u`.

6 In the **y-component** text field, type `0`.

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

8 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Magnitude controlled**.

9 In the **Minimum density level** text field, type `7.2`.

10 In the **Maximum density level** text field, type `10.9`.

11 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

12 In the **Tube radius expression** text field, type `0.05[mm]`.

13 Select the **Radius scale factor** checkbox.

14 Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

15 Select the **Number of arrows** checkbox. In the associated text field, type `100`.

16 Select the **Scale factor** checkbox. In the associated text field, type `0.0025`.

Color Expression 1

1 Right-click **Streamline Surface 1** and choose **Color Expression**.

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

3 In the **Expression** text field, type `tcs.p_wA`.

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

5 In the **Acetone Mass Fraction and Partial Pressure** toolbar, click **Plot**.

Finally, delete result nodes that are not needed, and group the remaining ones.

Moving Mesh 1, Pressure (spf) 1, Temperature (ht), Vapor Pressure, A, 3D (tcs), Vapor Pressure, N (tcs), Vapor Pressure, N, 3D (tcs), Vapor Pressure, W (tcs), Vapor Pressure, W, 3D (tcs), Velocity, 3D (spf) 1

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Vapor Pressure, W (tcs)**, **Vapor Pressure, W, 3D (tcs)**, **Vapor Pressure, N (tcs)**, **Vapor Pressure, N, 3D (tcs)**, **Vapor Pressure, A, 3D (tcs)**, **Pressure (spf) 1**, **Velocity, 3D (spf) 1**, **Temperature (ht)**, and **Moving Mesh 1**.

2 Right-click and choose **Delete**.

Acetone Mass Fraction and Partial Pressure

In the **Model Builder** window, collapse the **Results** > **Acetone Mass Fraction and Partial Pressure** node.

Acetone, Acetone Mass Fraction and Partial Pressure, Density, Droplet Shrinkage, Droplet Temperature, Evaporation Rate, Temperature, Vapor and Liquid Flow, Water

1. In the **Model Builder** window, under **Results**, Ctrl-click to select **Acetone**, **Vapor and Liquid Flow**, **Temperature**, **Density**, **Water**, **Evaporation Rate**, **Droplet Temperature**, **Droplet Shrinkage**, and **Acetone Mass Fraction and Partial Pressure**.
2. Right-click and choose **Group**.

Evaporation

In the **Settings** window for **Group**, type `Evaporation` in the **Label** text field.