



Vacuum Drying

Introduction

Vacuum drying is a chemical process frequently used in the pharmaceutical and food industries to remove water or an organic solvent from a wet powder. When designing a vacuum drying system, engineers aim to minimize the drying time while maintaining high quality in the product. This model investigates vacuum drying in a Nutsche filter-dryer, which consists of a cylindrical drum filled with wet cake as seen in [Figure 1](#). The top of the cake is exposed to a low pressure head space, and the side and bottom walls are exposed to heating fluid. By operating at a very low pressure and an elevated temperature, the evaporation rate of the liquid increases, thus accelerating the drying process of the powder. By modeling the heat transfer and evaporation of the solvent in the powder, the temperature and liquid phase profiles can be studied.

This example is based on the paper published by Murru and others for a powder dried with n-propanol under static conditions ([Ref. 1](#)).

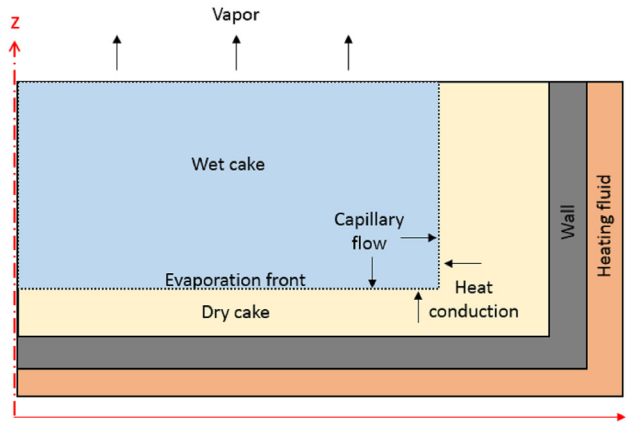


Figure 1: Vacuum drying in an axisymmetric Nutsche filter dryer ([Ref. 1](#)).

Model Definition

The cylindrical cake can be modeled using a rectangular geometry in a 2D axisymmetric component. The cake radius is 40 cm and the cake height is 10 cm.

The vacuum drying process involves heat transfer and vapor transport in modeling the evaporation of the solvent. This example simulates the heat transfer through the cake using the Heat Transfer in Solids interface and the volume fraction of solvent using a Coefficient

Form PDE interface. A predefined moisture transport in porous media physics interface is available in the Heat Transfer Module.

Heat flux boundary conditions are defined on the side and bottom boundaries to account for the external heating fluid. The evaporation of solvent is captured in two ways: a heat sink term to account for the energy lost from the cake as the liquid solvent changes to vapor phase, and a mass sink term to account for the loss of solvent in the cake.

LIQUID PHASE EVAPORATION

The equation in the Coefficient Form PDE interface solves for the volume fraction of liquid, θ_L , in the cake:

$$\frac{\partial \theta_L}{\partial t} = \nabla \cdot (D_L \nabla \theta_L) - \frac{\dot{m}_{LG}}{\rho_L}$$

where D_L is the apparent liquid diffusion coefficient, \dot{m}_{LG} is the evaporation rate, and ρ_L is the liquid phase density.

The source term \dot{m}_{LG}/ρ_L accounts for the loss of solvent as it evaporates. All boundaries are prescribed as no flux conditions.

The evaporation rate \dot{m}_{LG} is related to the difference in the equilibrium vapor pressure of the gas in the cake p^* and head space vapor pressure p_G with:

$$\dot{m}_{LG} = k_{\text{vap}} \rho_L (p^* - p_G) / p_G, \text{ if } \theta_L > 0$$

$$\dot{m}_{LG} = 0, \text{ if } \theta_L < 0 \text{ or } p^* \leq p_G$$

where k_{vap} is the evaporation rate constant (1/s). In this case, the head space pressure, or the vacuum pressure surrounding the cake, is set to be 15 mbar.

Evaporation should cease once the value of liquid phase reaches zero (fully evaporated) or if the local vapor pressure does not exceed the head space vapor pressure (no driving force for the evaporation). In the model, step functions are used to smoothly ramp the evaporation rate down to zero under these conditions.

The equilibrium vapor pressure of n-propanol, which is related to the temperature (T), can be found using Antoine's equation: $p^* = 10^{A - B/(C + T)}$ where A, B, and C are constants found in [Ref. 2](#).

The solvent migrates in the cake due to capillary flow. Instead of directly solving for the velocity field of the liquid phase in the porous media, the transport of the solvent through the cake can be approximated as a diffusion process. Therefore, when there is a gradient

in the volume fraction of solvent, the liquid phase migrates from the region with a high volume fraction of solvent to the region with a low volume fraction of solvent. The liquid diffusion coefficient is calculated with:

$$D_L = \alpha(\theta_L - \theta_L^*), \text{ if } \theta_L \geq \theta_L^*$$

$$D_L = 0, \text{ if } \theta_L < \theta_L^*$$

where θ_L^* is the residual saturation and α is the proportionality constant, both of which are determined experimentally in [Ref. 1](#). When the volume fraction of liquid phase present is below the critical value of θ_L^* , then diffusion of the solvent in the cake should no longer occur. In the model, a step function is used to smoothly ramp the diffusion coefficient down to zero under these conditions.

As the cake dries, the liquid phase evaporates and is replaced by gas between the solid particulates. The sum of the volume fractions of the three phases should equal unity. Therefore, the volume fraction of gas present (θ_G) can be calculated with respect to the constant volume fraction of solid powder (θ_S) and the variable liquid volume fraction (θ_L) with $\theta_G = 1 - (\theta_L + \theta_S)$.

HEAT TRANSFER

The equations in the Heat Transfer in Solids interface solve for the temperature, T , in the cake:

$$\rho_{\text{eff}} c_{p, \text{eff}} \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_{\text{eff}} \nabla T) + Q$$

where ρ_{eff} is the density (SI unit: kg/m³), C_p is the heat capacity (SI unit: J/(kg*K)), λ_{eff} is the thermal conductivity (SI unit: W/(m*K)), and Q is the heat source (SI unit: W/m³).

Energy is required for evaporation to occur, which is characterized in a heat source domain condition with $Q = -\dot{m}_{LG} \Delta H_{vap}$, where ΔH is the latent heat of vaporization (SI unit: J/kg) found in [Ref. 3](#).

The side and bottom boundaries of the filter-dryer are exposed to a heating fluid. In this model, heat flux boundary conditions account for the energy transferred to the cake from 60°C heating fluid given a heat transfer coefficient of 10 W/(m²*K).

The cake consists of solid powder particulates, a liquid solvent, and a gas that fills the voids between the solid powder particulates. Therefore, the material properties of the cake must

take into account the properties of the 3 phases in proportion to their presence in the cake. In this case, the effective density ρ_{eff} and effective heat capacity $c_{p,\text{eff}}$ are calculated with:

$$\rho_{\text{eff}} = \theta_L \rho_L + \theta_S \rho_S + \theta_G \rho_G$$

$$c_{p,\text{eff}} = (\theta_L \rho_L c_{p,L} + \theta_S \rho_S c_{p,S} + \theta_G \rho_G c_{p,G}) / \rho_{\text{eff}}$$

where θ_L , θ_S , and θ_G represent the volume fraction of the liquid, solid, and gas phases in the cake, respectively. The material properties of the liquid phase (ρ_L and $c_{p,L}$) are taken from Ref. 4 for n-propanol at a temperature of 40°C. Solid powder properties are found in Ref. 1.

The effective thermal conductivity is calculated with:

$$\lambda_{\text{eff}} = \lambda_{\text{dry}} + \frac{\theta_L}{1 - \theta_S} (\lambda_{\text{wet}} - \lambda_{\text{dry}})$$

where λ_{dry} and λ_{wet} are the thermal conductivities of the dry and fully saturated cake, respectively, found in Ref. 1. Instead of writing user defined expressions for the effective material properties of the cake, the **Multiphase Material** is used.

Results and Discussion

The following figures show the temperature (Figure 2), volume fraction of liquid phase (Figure 3), and the apparent moisture diffusivity (Figure 4) in the cake after 30 hours. The temperature of the cake approaches the temperature of the heating fluid (60°C or 333.15 K) at the bottom and side boundaries, as seen in Figure 2. Because the liquid phase evaporates in the heated region, the volume fraction of the liquid phase is lowest near the heated side and bottom boundaries and highest in the center of the cake, as seen in Figure 3. The apparent moisture diffusivity is also highest in the center of the cake where liquid phase has not yet evaporated and approaches zero in areas where the liquid phase has already evaporated, as seen in Figure 4.

The evaporation rate after 10, 20, and 30 hours is shown in Figure 5, Figure 6, and Figure 7. The evaporation front starts near the side and bottom walls where the cake is heated. As the amount of solvent present near these boundaries decreases, the evaporation rate decreases in turn, shifting the evaporation front toward the center of the cake.

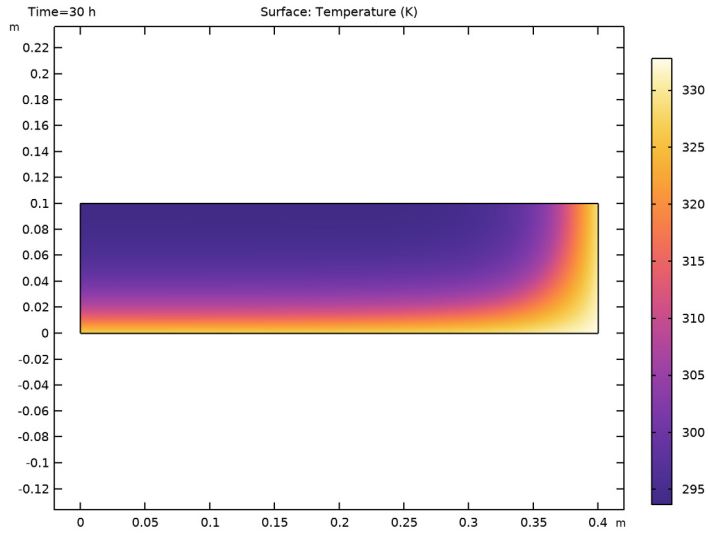


Figure 2: Temperature in the cake after 30 hours.

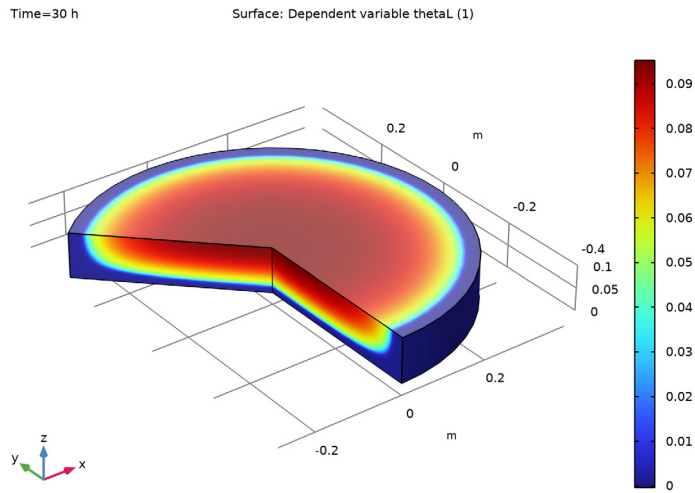


Figure 3: Volume fraction of liquid phase in the cake after 30 hours.

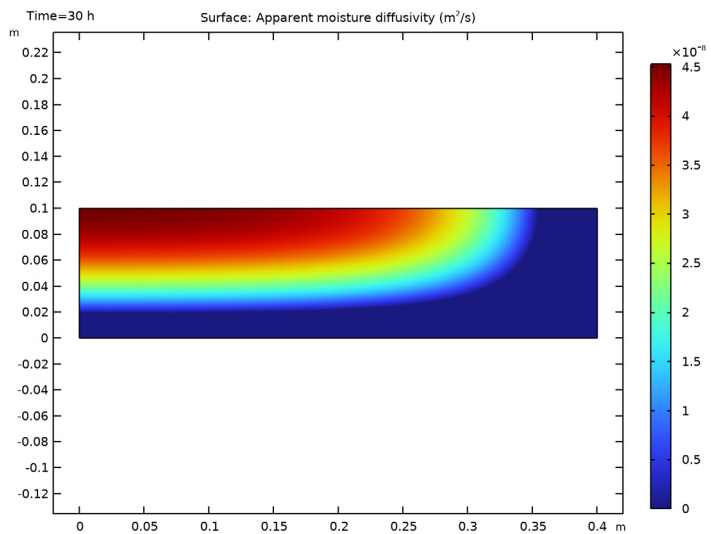


Figure 4: Apparent moisture diffusivity in the cake after 30 hours.

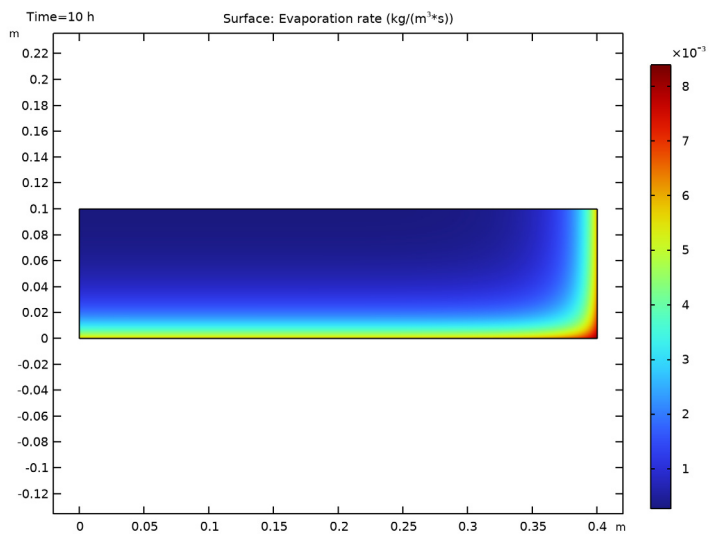


Figure 5: Evaporation rate after 10 hours.

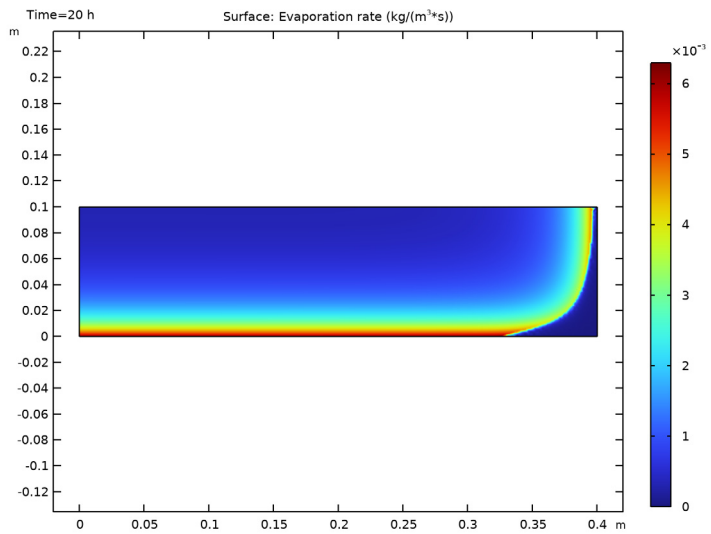


Figure 6: Evaporation rate after 20 hours.

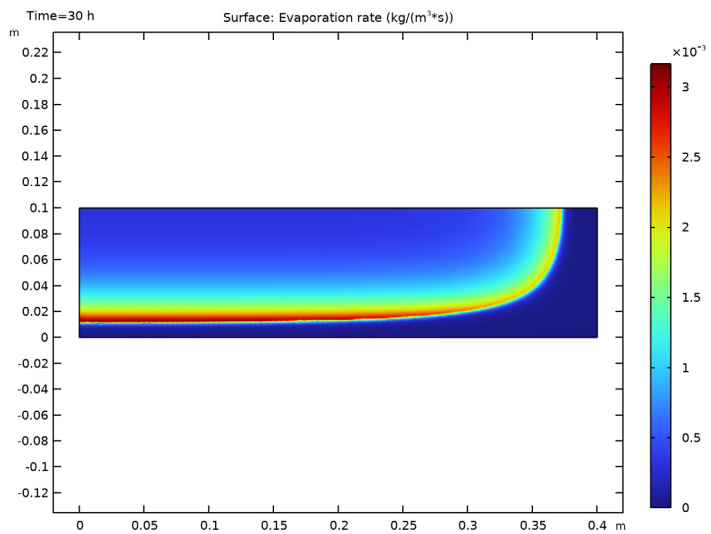


Figure 7: Evaporation rate after 30 hours.

References


1. M. Murru and others, “Model-based scale-up of vacuum contact drying of pharmaceutical compounds,” *Chem. Eng. Sci.*, vol. 66, pp. 5045–5054, 2011.
 2. H.R. Kemme and S.I. Kreps, “Vapor pressure of primary n-alkyl chlorides and alcohols”, *J. Chem. Eng. Data*, vol. 14, no. 1, pp. 98–102. 1969.
 3. I.M. Smallwood, *Handbook of Organic Solvent Properties*, Arnold, 1996.
 4. “n-Propanol”, BASF, Technical Leaflet, March 2008.
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Application Library path: COMSOL_Multiphysics/Chemical_Engineering/vacuum_drying

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

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

3 Click **Add**.

Add also a PDE interface to solve for the volume fraction of liquid in the cake.

4 In the **Select Physics** tree, select **Mathematics>PDE Interfaces>Coefficient Form PDE (c)**.

5 Click **Add**.

6 In the **Field name (I)** text field, type `theta`.

7 In the **Dependent variables (I)** table, enter the following settings:

<code>thetaL</code>

8 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	1/s

9 Click  **Study**.

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

11 Click  **Done**.

The list of parameters and variables are imported from files available in the Application Libraries folder.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 Click  **Load from File**.

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

DEFINITIONS

Variables 1

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

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

3 Click  **Load from File**.

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

Next define two step functions to smoothly decrease the evaporation rate and apparent moisture diffusivity to zero as the solvent evaporates.

Step 1 (step1)

1 In the **Home** toolbar, click  **Functions** and choose **Global>Step**.

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

3 In the **Location** text field, type 1.005.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type 0.01.

Step 2 (step2)



1 In the **Home** toolbar, click  **Functions** and choose **Global>Step**.

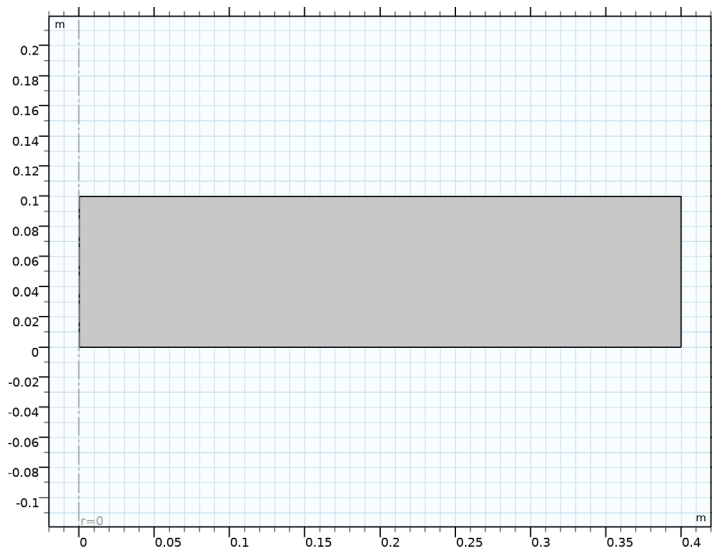
2 In the **Settings** window for **Step**, locate the **Parameters** section.

- 3 In the **Location** text field, type 0.005.
- 4 Locate the **Smoothing** section. In the **Size of transition zone** text field, type 0.01.

GEOMETRY I

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 R0.
- 4 In the **Height** text field, type H0.
- 5 Click  **Build All Objects**.



MATERIALS

Multiphase Material 1 (mpmat1)

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **More Materials>Multiphase Material**.

Constrained Gas Phase

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Materials>Multiphase Material 1 (mpmat1)** click **Phase 1 (mpmat1.phase1)**.
- 2 In the **Settings** window for **Phase**, type Constrained Gas Phase in the **Label** text field.

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_{iso} ; $k_{ij} = k_{iso}$, $k_{ij} = 0$	$\lambda_{dry} / (1 - \theta_S)$	W/(m·K)	Basic
Density	ρ	ρ_G	kg/m ³	Basic
Heat capacity at constant pressure	C_p	C_{pG}	J/(kg·K)	Basic

Liquid Phase

1 In the **Model Builder** window, right-click **Multiphase Material 1 (mpmat1)** and choose **Phase**.

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

3 Locate the **Volume Fraction** section. In the V_f text field, type $\theta_{L,S}$.

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_{iso} ; $k_{ij} = k_{iso}$, $k_{ij} = 0$	$\lambda_{wet} / (1 - \theta_S)$	W/(m·K)	Basic
Density	ρ	ρ_L	kg/m ³	Basic
Heat capacity at constant pressure	C_p	C_{pL}	J/(kg·K)	Basic

Solid Phase

1 Right-click **Multiphase Material 1 (mpmat1)** and choose **Phase**.

2 In the **Settings** window for **Phase**, type Solid Phase in the **Label** text field.

3 Locate the **Volume Fraction** section. In the V_f text field, type $\theta_{L,S}$.

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

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_{iso} ; $k_{ij} = k_{iso}$, $k_{ij} = 0$	0	W/(m·K)	Basic


Property	Variable	Value	Unit	Property group
Density	rho	rhoS	kg/m ³	Basic
Heat capacity at constant pressure	Cp	CpS	J/(kg·K)	Basic

HEAT TRANSFER IN SOLIDS (HT)

Heat Source 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Heat Transfer in Solids (ht)** and choose **Heat Source**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.
- 4 In the Q_0 text field, type $-\dot{m} \cdot \Delta H$.

Heat Flux 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Heat Flux**.
- 2 Select Boundaries 2 and 4 only.
- 3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.
- 4 From the **Flux type** list, choose **Convective heat flux**.
- 5 In the h text field, type h_q .
- 6 In the T_{ext} text field, type T_h .

Initial Values 1

- 1 In the **Model Builder** window, click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the T text field, type T_0 .

Next, define the Coefficient Form PDE interface for the liquid phase evaporation.

COEFFICIENT FORM PDE (C)

Coefficient Form PDE 1


- 1 In the **Model Builder** window, under **Component 1 (comp1)**>**Coefficient Form PDE (c)** click **Coefficient Form PDE 1**.
- 2 In the **Settings** window for **Coefficient Form PDE**, locate the **Diffusion Coefficient** section.
- 3 In the c text field, type DL .
- 4 Locate the **Source Term** section. In the f text field, type $-\dot{m} / \rho_{\text{H}_2\text{O}}$.

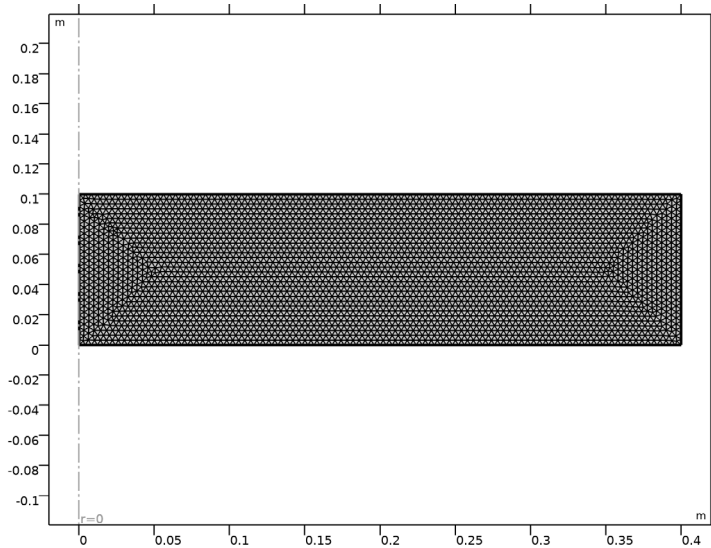
Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the *thetaL* text field, type thetaL0.

Set the mesh to extremely fine to better resolve the evaporation front in the domain.

MESH I

- 1 In the **Model Builder** window, under **Component I (comp1)** click **Mesh I**.
- 2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.
- 3 From the **Element size** list, choose **Extremely fine**.
- 4 Click  **Build All**.



STUDY I

Solution I (sol1)


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

The dependent variable scaling for thetaL is manually set to 1. This provides a better convergence.

- 2 In the **Model Builder** window, expand the **Solution I (sol1)** node.


- 3 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** node, then click **Dependent variable thetaL (comp1.thetaL)**.
- 4 In the **Settings** window for **Field**, locate the **Scaling** section.
- 5 From the **Method** list, choose **Manual**.

Step 1: Time Dependent


- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **h**.
- 4 In the **Output times** text field, type range(0,1,70).
- 5 In the **Study** toolbar, click  **Compute**.

RESULTS

Coefficient Form PDE 1


- 1 In the **Model Builder** window, under **Results** click **Coefficient Form PDE 1**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.
- 3 From the **Time (h)** list, choose **30**.
- 4 In the **Coefficient Form PDE 1** toolbar, click  **Plot**.

ADD PREDEFINED PLOT

- 1 In the **Home** toolbar, click  **Windows** and choose **Add Predefined Plot**.
- 2 Go to the **Add Predefined Plot** window.
- 3 In the tree, select **Study 1/Solution 1 (sol1)>Heat Transfer in Solids>Temperature (ht)**.
- 4 Click **Add Plot** in the window toolbar.

RESULTS

Apparent moisture diffusivity

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type Apparent moisture diffusivity in the **Label** text field.
- 3 Locate the **Data** section. From the **Time (h)** list, choose **30**.

Surface 1

- 1 Right-click **Apparent moisture diffusivity** and choose **Surface**.

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

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

4 In the **Apparent moisture diffusivity** toolbar, click  **Plot**.

Evaporation rate

1 In the **Home** toolbar, click  **Add Plot Group** and choose **2D Plot Group**.

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


3 Locate the **Data** section. From the **Time (h)** list, choose **30**.

Surface I

1 Right-click **Evaporation rate** and choose **Surface**.

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

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

4 In the **Evaporation rate** toolbar, click  **Plot**.