Model created in COMSOL Multiphysics 6.4

Stefan Tube

Introduction

This example illustrates the use of the Maxwell-Stefan diffusion model available with the Transport of Concentrated Species interface. It models multicomponent gas-phase diffusion in a Stefan tube in 1D. In this case, it is a liquid mixture of acetone and methanol that evaporates into air.

The concentration profiles are modeled at steady-state and validated against experimental data by Taylor and Krishna (Ref. 6).

Model Definition

The Stefan tube, shown in Figure 1, is a simple device used for measuring diffusion coefficients in binary vapors.

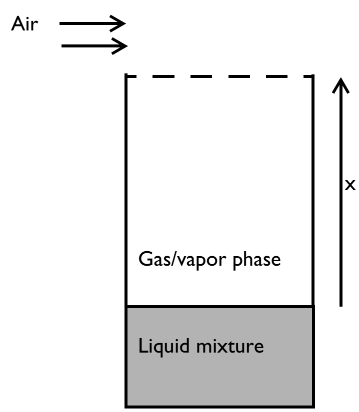

Figure 1: Schematic diagram of a Stefan tube.

At the bottom of the tube is a pool of mixture. The vapor that evaporates from this pool diffuses to the top of the tube, where a stream of air, flowing across the top of the tube, keeps the mole fraction of diffusing vapor there to be zero. The mole fraction of vapor above the liquid interface is at equilibrium. Because there is no horizontal flux inside the tube, you can analyze the problem using a 1D model geometry representing the distance between the liquid mixture surface and the top of the tube. The system composition of acetone, methanol, and air has been extensively investigated; both diffusion coefficients and composition have been measured at various positions within Stefan tubes. This makes it an ideal system for this model.

As a comparison, one experiment measured the mole fraction at the liquid interface to be $x_{Ac} = 0.319$ and $x_{Me} = 0.528$ where the pressure, p, was 99.4 kPa and the temperature, T, was 328.5 K. The length of the diffusion path was 0.238 m. The respective Maxwell-Stefan diffusion coefficients, D_{ij}, of the three binary pairs were calculated and are used in the model according to Table 1.

TABLE 1: LABELS AND MAXWELL-STEFAN DIFFUSION COEFFICIENTS.

COMPONENT	LABEL	D_{ij}	VALUE
Acetone	1	D_{12}	$8.48\cdot10^{-6}$ m^2/s
Methanol	2	D_{13}	$13.72\cdot10^{-6}$ m^2/s
Air	3	D_{23}	$19.91\cdot10^{-6}$ m^2/s

To model this problem, use the Transport of Concentrated Species interface with the Maxwell-Stefan diffusion model. It solves for the fluxes in terms of mass fractions for two of the three components. The mass fraction of the third, ω_3, is given by the two other ones. The three governing equations are

$$\nabla\cdot\left[-\rho\omega_1\sum_k D_{1k}\left[\nabla x_k+(x_k-\omega_k)\frac{\nabla p_A}{p_A}\right]+D_1^T\left(\frac{\nabla T}{T}\right)\right] = R_1-\rho(\mathbf{u}\cdot\nabla)\omega_1$$

$$\nabla\cdot\left[-\rho\omega_2\sum_k D_{2k}\left[\nabla x_k+(x_k-\omega_k)\frac{\nabla p_A}{p_A}\right]+D_2^T\left(\frac{\nabla T}{T}\right)\right] = R_2-\rho(\mathbf{u}\cdot\nabla)\omega_2$$

$$\omega_3 = 1-\omega_1-\omega_2$$

where D_{ij} are the multicomponent Fick diffusivities (SI unit: m^2/s), p_A is the absolute pressure (SI unit: Pa), T is the temperature (SI unit: K), D_i^T is the thermal diffusion coefficient (SI unit: kg/(m·s)), and $\mathbf{u}$ is the mixture averaged velocity (SI unit: m/s). Species mole fractions and mass fractions are denoted by x and ω respectively, and the mixture density, ρ (SI unit: kg/m^3), is a function of the average mixture mole fraction, M_{mix} (SI unit: kg/mol), according to Equation 2:

$$M_{mix} = \sum_i x_i M_i \tag{1}$$

$$\rho = \frac{p}{RT}M_{mix} \tag{2}$$

In this case, there is no imposed fluid velocity. However, a mixture velocity will result due to the mass transfer from liquid mixture. At the top of the tube the mass fractions are fixed, with the fraction of air being unity. At the bottom (at the liquid interface), the fractions are also fixed according to the previously mentioned experimental conditions. The fact that there is no air flux at the interface results in the following relation for the convective velocity, at steady state:

$$u = \frac{j_{\mathrm{diff},3}}{\omega_3 \rho}$$

where $j_{\mathrm{diff},3}$ is the diffusive mass flux of air (SI unit: $\mathrm{kg/(m^2 \cdot s)}$).

Results

Both the modeled and experimental steady-state mole fractions as a function of position are shown in Figure 2.

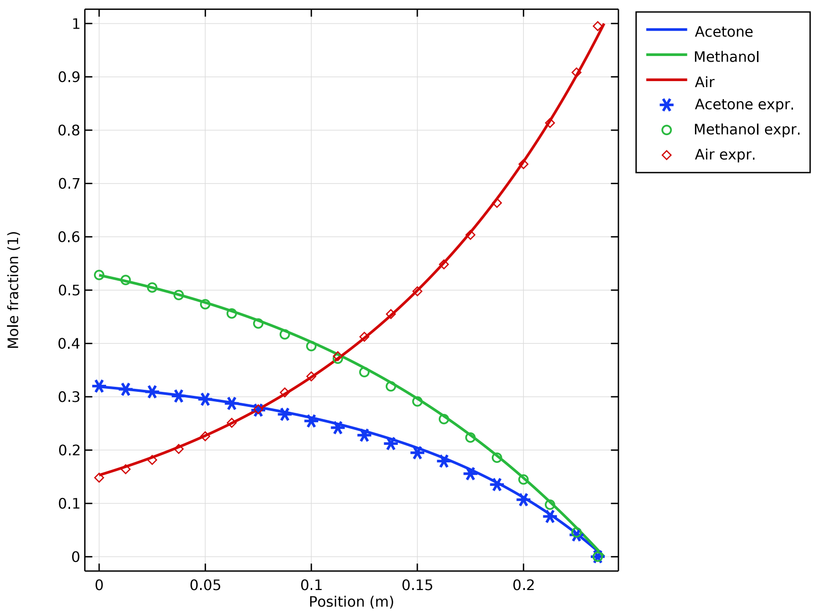

Figure 2: Modeled and experimental (Ref. 6) steady-state mole fractions of: acetone, methanol, and air, in the Stefan tube.

We can see that the model reproduces the results from Ref. 6 well, which means the Maxwell-Stefan equations can describe the mass transport process in the system accurately.

The Maxwell-Stefan diffusion formulation includes the conservation of mass. In the absence of chemical reactions (source terms) and convective contributions, the Maxwell-

Stefan formulation results in zero net mass flux. In this example, the convective term is included, which you can see in the velocity profile in Figure 3.

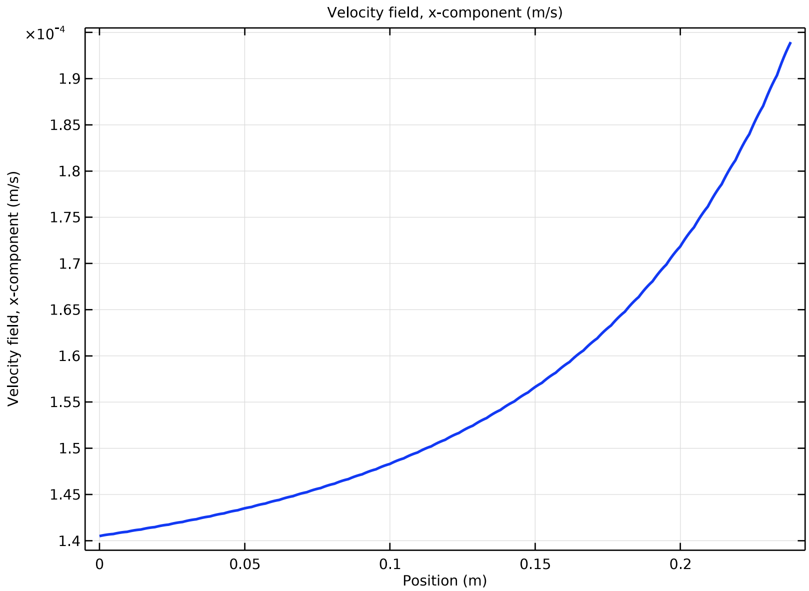

Figure 3: Velocity of the gas mixture in the Stefan tube.

References

1. C.F. Curtiss and R.B. Bird, "Multicomponent diffusion," *Ind. Eng. Chem. Res.*, vol. 38, p. 2515, 1999.

2. R.B. Bird, W. Stewart, and E. Lightfoot, *Transport Phenomena*, John Wiley & Sons, New York, 1960.

3. G.A.J. Jaumann, *Wien. Akad. Sitzungsberichte (Math.-Naturw. Klasse)*, vol. 120, p. 385, 1911.

4. J.O. Hirschfelder, C.F. Curtiss, and R.B. Bird, *Molecular Theory of Gases and Liquids*, Wiley, USA, 1954.

5. E.N. Fuller, P.D. Schettler, and J.C. Giddings, *Ind. Eng. Chem.*, vol. 58, p. 19, 1966.

6. R. Taylor and R. Krishna, *Multicomponent Mass Transfer,* John Wiley & Sons, NY, p. 21, 1993.

Application Library path: `Chemical_Reaction_Engineering_Module/Mixing_and_Separation/stefan_tube`

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 **1D**.

2 In the **Select Physics** tree, select **Chemical Species Transport** > **Transport of Concentrated Species (tcs)**.

3 Click **Add**.

4 Click **Add Mass Fraction**.

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

w1
w2
w3

6 Click **Study**.

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

8 Click **Done**.

GLOBAL DEFINITIONS

Next, add a set of model parameters by importing their definitions from a data text file provided with the **Application Library**.

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 `stefan_tube_parameters.txt`.

GEOMETRY 1

Interval 1 (i1)

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

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

3 In the table, enter the following settings:

Coordinates (m)
0
0.238

4 Click **Build All Objects**.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

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

2 In the **Settings** window for **Transport of Concentrated Species**, locate the **Transport Mechanisms** section.

3 From the **Diffusion model** list, choose **Maxwell–Stefan**.

4 Locate the **Species** section. From the **From mass constraint** list, choose **w3**.

5 Click to expand the **Discretization** section. From the **Mass fraction** list, choose **Quadratic**.

Species Molar Masses 1

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

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 In the M_{w1} text field, type `M_ace`.

4 In the M_{w2} text field, type `M_met`.

5 In the M_{w3} text field, type `M_air`.

Fluid 1

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

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

3 From the T list, choose **User defined**. In the associated text field, type `T0`.

4 From the p_A list, choose **User defined**. In the associated text field, type `p0`.

5 Locate the **Convection** section. Specify the **u** vector as

`-tcs.dflux_w3x/(w3*tcs.rho)`	x

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

Species 1	Species 2	Diffusivity	Diffusion coefficient (m^2/s)
w1	w2	User defined	D12
w1	w3	User defined	D13
w2	w3	User defined	D23

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 $\omega_{0,\mathrm{w1}}$ text field, type `w_ace0`.

4 In the $\omega_{0,\mathrm{w2}}$ text field, type `w_met0`.

Mass Fraction 1

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

2 Select Boundary 1 only.

3 In the **Settings** window for **Mass Fraction**, locate the **Mass Fraction** section.

4 Select the **Species w1** checkbox.

5 In the $\omega_{0,\mathrm{w1}}$ text field, type `w_ace0`.

6 Select the **Species w2** checkbox.

7 In the $\omega_{0,\mathrm{w2}}$ text field, type `w_met0`.

Mass Fraction 2

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

2 Select Boundary 2 only.

3 In the **Settings** window for **Mass Fraction**, locate the **Mass Fraction** section.

4 Select the **Species w1** checkbox.

5 Select the **Species w2** checkbox.

MESH 1

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

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

3 From the **Element size** list, choose **Extra fine**.

4 Click **Build All**.

STUDY 1

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

RESULTS

Experimental Mole Fractions

1 In the **Results** toolbar, click **Table**.

Import the experimental data for comparison.

2 In the **Settings** window for **Table**, type `Experimental Mole Fractions` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

In order to reproduce the plot in Figure 2, do the following:

Mole Fractions Compared with Experimental Data

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

2 In the **Settings** window for **1D Plot Group**, type `Mole Fractions Compared with Experimental Data` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **x-axis label** checkbox. In the associated text field, type `Position (m)`.

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

Line Graph 1

1 Right-click **Mole Fractions Compared with Experimental Data** and choose **Line Graph**.

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

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

4 Click to expand the **Title** section. Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species** > **Species w1** > **tcs.x_w1 - Mole fraction - 1**.

5 Locate the **Title** section. From the **Title type** list, choose **None**.

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

7 In the **Expression** text field, type `x`.

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

9 Click to expand the **Legends** section. Select the **Show legends** checkbox.

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

11 In the table, enter the following settings:

Legends
Acetone

Line Graph 2

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

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species** > **Species w2** > **tcs.x_w2 - Mole fraction - 1**.

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

Legends
Methanol

Line Graph 3

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

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species** > **Species w3** > **tcs.x_w3 - Mole fraction - 1**.

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

Legends
Air

Table Graph 1

1 In the **Model Builder** window, right-click **Mole Fractions Compared with Experimental Data** and choose **Table Graph**.

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

3 From the **x-axis data** list, choose **Distance from surface (m)**.

4 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

5 Find the **Line style** subsection. From the **Line** list, choose **None**.

6 From the **Color** list, choose **Cycle (reset)**.

7 Click to expand the **Legends** section. Select the **Show legends** checkbox.

8 Find the **Prefix and suffix** subsection. In the **Suffix** text field, type `expr.`.

Use a **Comparison** node to quantify the difference between the computed mole fractions and the experimental data.

Comparison 1

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

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

3 From the **Column** list, choose **Acetone**.

4 Locate the **Comparison** section. From the **Metric** list, choose **RMS**.

5 In the **Mole Fractions Compared with Experimental Data** toolbar, click **Plot**.

Comparison 1

1 In the **Model Builder** window, right-click **Line Graph 2** and choose **Comparison**.

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

3 From the **Column** list, choose **Methanol**.

4 Locate the **Comparison** section. From the **Metric** list, choose **RMS**.

5 In the **Mole Fractions Compared with Experimental Data** toolbar, click **Plot**.

Comparison 1

1 In the **Model Builder** window, right-click **Line Graph 3** and choose **Comparison**.

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

3 From the **Column** list, choose **Air**.

4 Locate the **Comparison** section. From the **Metric** list, choose **RMS**.

5 In the **Mole Fractions Compared with Experimental Data** toolbar, click **Plot**.

   It can be noted that the root-mean square difference for all three mole fractions is around 0.006.

To reproduce Figure 3, proceed as follows:

Velocity Field

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

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

3 Locate the **Plot Settings** section.

4 Select the **x-axis label** checkbox. In the associated text field, type `Position (m)`.

Line Graph 1

1. Right-click **Velocity Field** and choose **Line Graph**.
2. Select Domain 1 only.
3. In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Transport of Concentrated Species** > **Velocity field - m/s** > **tcs.u - Velocity field, x-component**.
4. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
5. In the **Expression** text field, type x.
6. Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
7. In the **Velocity Field** toolbar, click **Plot**.