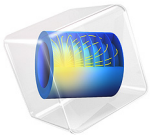

Electroosmotic Flow in Porous Media

Introduction

This example treats the modeling of electroosmotic flow in porous media (Ref. 1, Ref. 2). The system consists of a compartment of sintered porous material and two electrodes that generate an electric field. The cell combines pressure-driven and electroosmotic flow.

The purpose of this example is to illustrate the modeling of electroosmosis and electrophoresis in porous media in COMSOL Multiphysics.

Model Definition

Figure 1 shows the system's geometry. It is made up of a domain of porous material containing the electrolyte and two electrodes that generate a potential difference. The conductivity is very small, and the model assumes that the effects of electrochemical reactions at the electrode surfaces are negligible.

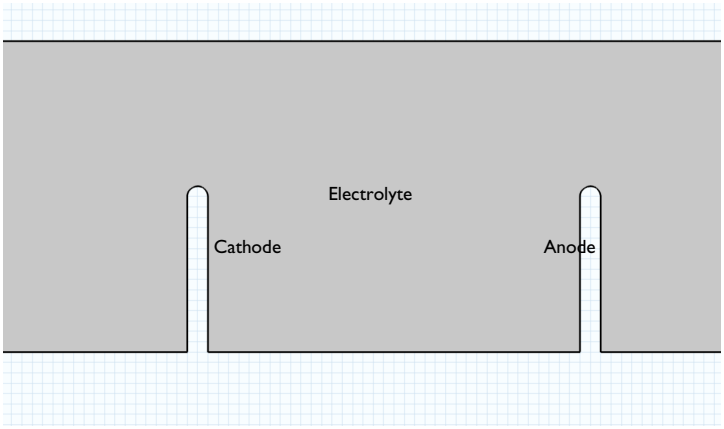

Figure 1: The modeled domain consists of an electrolyte contained in a porous structure and two electrodes that generate an electric field.

In the first part of the model, you solve the continuity equations for the flow velocity and the current density at steady state:

$$\nabla \cdot \mathbf{u} = 0$$
$$\nabla \cdot \mathbf{i} = 0$$

Here $\mathbf{u}$ denotes the velocity (SI unit: m/s) and $\mathbf{i}$ represents the current-density vector (SI unit: A/m^2). The velocity includes two driving forces — a pressure term and an electroosmotic term:

$$\mathbf{u} = -\frac{\varepsilon_p a^2}{8\mu\tau}\nabla p + \frac{\varepsilon_p \varepsilon_w \zeta}{\mu\tau}\nabla V$$

In this equation, ε_p denotes the porosity, a is the average radius of the pores (SI unit: m), μ gives the fluid's dynamic viscosity (SI unit: Pa·s), τ represents the tortuosity of the porous structure, ε_w is the fluid's permittivity (SI unit: F/m), p gives the pressure (SI unit: Pa), ζ is the zeta potential (SI unit: V), and V equals the potential (SI unit: V). This equation is solved with a General Form PDE interface. The current density is modeled with the Electric Currents interface and solves the following:

$$\mathbf{i} = -\kappa\nabla V$$

where κ denotes the conductivity (SI unit: S/m).

At the solid walls, the normal velocity component vanishes:

$$\mathbf{u} \cdot \mathbf{n} = 0$$

At the inlet and the outlet, the pressure is fixed.

The boundary conditions for the current-density balance are insulating for all boundaries except the electrode surfaces, where the potential is fixed:

$\mathbf{i} \cdot \mathbf{n} = 0$	(all boundaries except the electrodes)
$V = V_1$	(anode surface)
$V = 0$	(cathode surface)

In the second model stage, you use the steady-state velocity and potential fields in a transient simulation of the concentration of a charged tracer species injected into the system, assuming that the tracer species does not influence the conductivity or the set potential in the porous structure. The mass-transport equation for the tracer is solved with the Transport of Diluted Species interface and reads:

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{N} = 0 \tag{1}$$

where $\mathbf{N}$ is the flux vector given by the Nernst-Planck equation:

$$\mathbf{N} = -D\nabla c - z u_m F c \nabla V + c\mathbf{u}$$

In this equation, D denotes the tracer's diffusivity (SI unit: m^2/s), c gives its concentration (SI unit: mol/m^3), z represents the tracer's charge number, and F is Faraday's constant

(SI unit: C/mol). The mobility, u_m (SI unit: mol·m^2/(J·s)), is given by the Nernst-Einstein equation

$$u_m = \frac{D}{R_g T}$$

where R_g = 8.314 J/(mol·K) is the gas constant and T (SI unit: K) is the temperature.

The boundary conditions for Equation 1, the mass-transport equation, are insulating except at the inlet and the outlet. There you use the Flux condition to set the diffusive and convective contributions to the flux through the boundaries to zero:

$$\mathbf{n} \cdot (-D\nabla c + c\mathbf{u}) = 0 \qquad \text{(inlet and outlet)}$$
$$\mathbf{n} \cdot \mathbf{N} = 0 \qquad \text{(all other boundaries)}$$

The initial concentration is given by a distribution that is uniform in the y direction and bell-shaped in the x direction:

$$c(t{=}0) = c_{top} \exp\left(-0.5\left(\frac{(x - x_m)}{p_w}\right)^2\right)$$

Here c_{top} denotes the peak concentration, x_m is the position of the peak along the x-axis, and p_w equals the base width of the peak.

Results and Discussion

The upper plot in Figure 2 shows the flow distribution in the porous structure when only the electric field acts as a driving force. In the lower plot, it is instead the pressure gradient that drives the flow. In both cases, the velocity is large around the corners of the electrodes, where the field strength is large and the effect of the decrease in the geometry's cross section is most pronounced. A comparison of the maximum flow-velocity values shows that the pressure gradient is the dominating driving force.

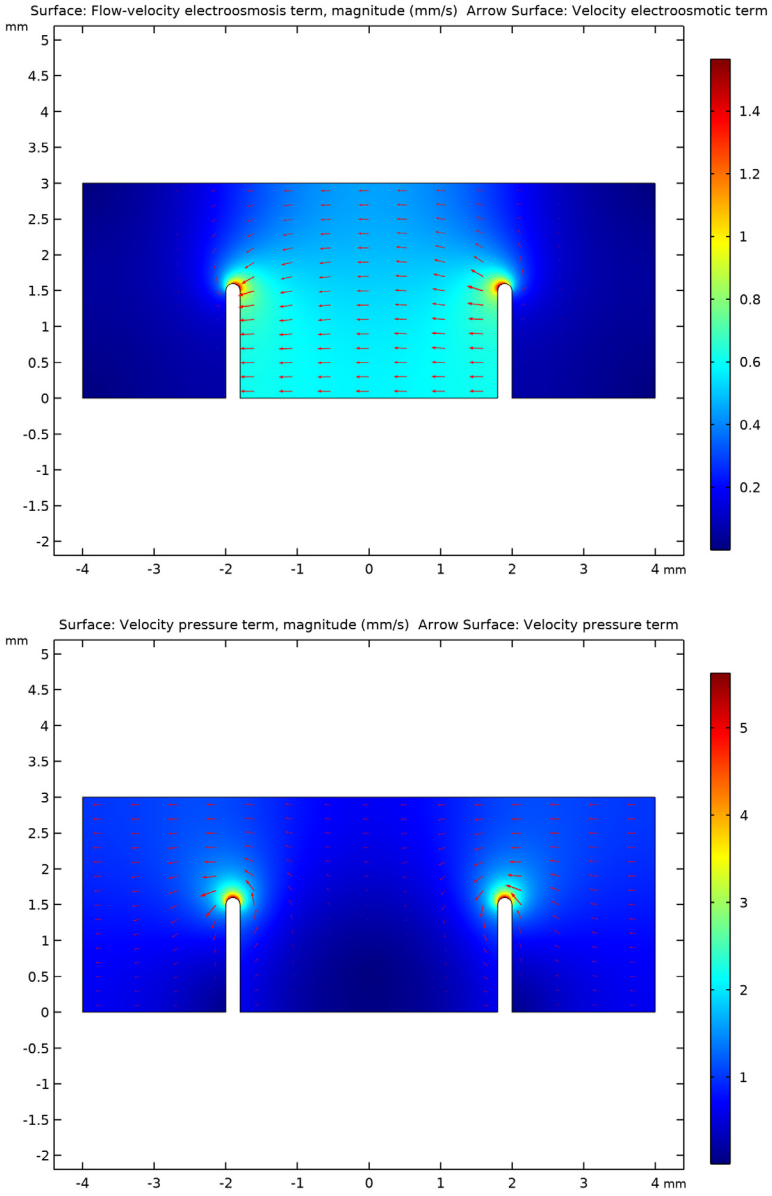

Figure 2: Velocity distributions in the cell with an applied electric field (top) and an applied pressure difference (bottom). The unit for the magnitude surface plot is mm/s.

Figure 3 shows the concentration field in the case where both pressure and electroosmotic forces are included. The figure shows that the migration of the charged tracer also influences the transport rate. In this case, the tracer is transported both by the movement of the flow, due to pressure and electroosmotic terms, and the electrophoretic effect on the charged tracer itself. At $t = 0$, the tracer is introduced as a bell-shaped vertical distribution near the inlet. In the subsequent simulation, this distribution is sheared and transported by diffusion, migration, and convection.

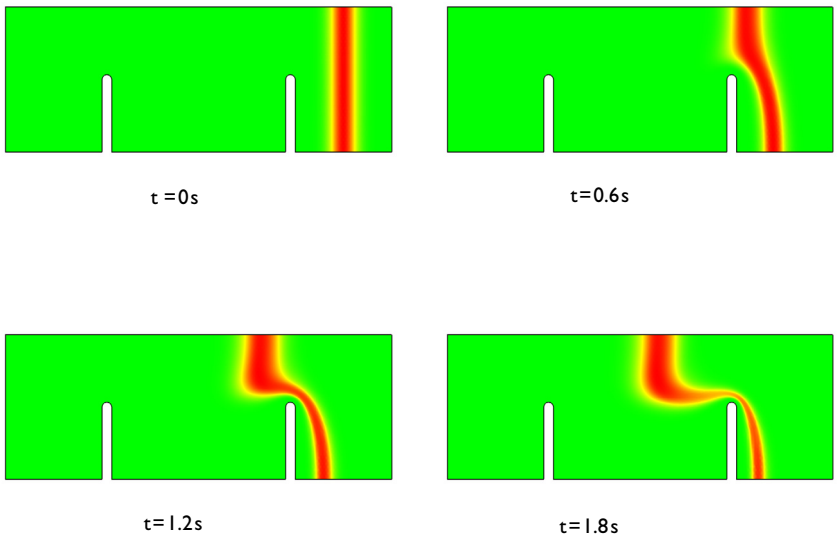

Figure 3: Concentration distribution in the domain at different times after injection. The effects of diffusion, convection, and migration deform the initial bell-shaped pulse.

Figure 4 shows the cross sections of the pulse along a line at $y = 2.5$ mm for the times $t = 0$, 0.5 s, 1.0 s, 1.5 s, and $t = 2.0$ s. Diffusion, mainly numerical diffusion, smears out the

pulse, while migration and convection mainly translate and shear it, depending on the pressure and the electric field.

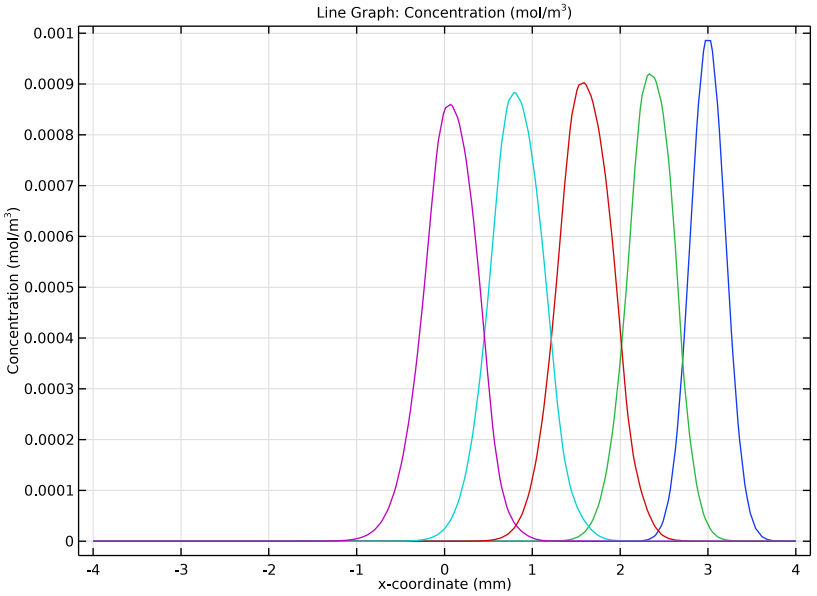

Figure 4: Cross-section plot of the concentration along a horizontal line at y = 2.5 mm for the times t = 0 (blue solid), 0.5 s, 1.0 s, 1.5 s, and 2.0 s.

Despite its geometrical simplicity, this example includes the components needed to model complex-shaped domains.

References

1. M-S. Chun, "Electrokinetic Flow Velocity in Charged Slit-like Microfluidic Channels with Linearized Poisson-Boltzmann Field," *Korean J. Chem. Eng.*, vol. 19, no. 5, pp. 729–734, 2002.

2. S. Yao, D. Huber, J. Mikkelsen, and J.G. Santiago, "A Large Flowrate Electroosmotic Pump with Micron Pores," *Proc. IMECE, 2001 ASME International Mechanical Engineering Congress and Exposition*, New York, November 2001.

Notes About the COMSOL Implementation

The COMSOL Multiphysics implementation is straightforward, and the only aspect to remember is to solve the steady-state problem first and then the time-dependent problem.

Application Library path: `Chemical_Reaction_Engineering_Module/Electrokinetic_Effects/electroosmotic_flow`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **AC/DC>Electric Fields and Currents>Electric Currents (ec)**.

3 Click **Add**.

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

5 Click **Add**.

6 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species (tds)**.

7 Click **Add**.

8 Click **Study**.

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

10 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

For your convenience, parameters and variables are made available in text files.

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 `electroosmotic_flow_parameters.txt`.

In these expressions, the predefined physical constants `epsilon0_const` and `R_const` refer to the permittivity of vacuum and the gas constant, respectively.

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **Local 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 `electroosmotic_flow_variables.txt`.

GEOMETRY 1

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

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

Now create the geometry. To simplify this step, insert the geometry sequence directly from the model's Application Libraries file:

4 In the **Geometry** toolbar, click **Insert Sequence**.

5 Browse to the model's Application Libraries folder and double-click the file `electroosmotic_flow.mph`.

Rectangle 1 (r1)

Make all the necessary geometry selections.

Cathode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **dif1**, select Boundaries 4, 5, 11, and 12 only.

Anode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **dif1**, select Boundaries 7, 8, 13, and 14 only.

Inlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **dif1**, select Boundary 1 only.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **dif1**, select Boundary 10 only.

In the Electric Currents interface set the electrolyte properties to compute the current density within the device.

ELECTRIC CURRENTS (EC)

Current Conservation 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Electric Currents (ec)** click **Current Conservation 1**.

2 In the **Settings** window for **Current Conservation**, locate the **Constitutive Relation Jc-E** section.

3 From the σ list, choose **User defined**. In the associated text field, type `kappa0`.

4 Locate the **Constitutive Relation D-E** section. From the ε_r list, choose **User defined**.

Electric Potential 1

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

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

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

Electric Potential 2

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

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

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

4 Locate the **Electric Potential** section. In the V_0 text field, type `V_anode`.

Continue with the General Form PDE interface and set up a convective velocity depending on pressure and electroosmosis. The dependent value is the pressure.

ELECTROOSMOTIC PRESSURE

1 In the **Model Builder** window, under **Component 1 (comp1)** click **General Form PDE (g)**.

2 In the **Settings** window for **General Form PDE**, type `Electroosmotic Pressure` in the **Label** text field.

3 Locate the **Units** section. Click  **Select Dependent Variable Quantity**.

4 In the **Physical Quantity** dialog box, type `pressure` in the text field.

5 Click  **Filter**.

6 In the tree, select **General>Pressure (Pa)**.

7 Click **OK**.

8 In the **Settings** window for **General Form PDE**, locate the **Units** section.

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

Source term quantity	Unit
Custom unit	1/s

10 Click to expand the **Dependent Variables** section. In the **Field name** text field, type `p`.

11 In the **Dependent variables** table, enter the following settings:

p

General Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Electroosmotic Pressure (g)** click **General Form PDE 1**.

2 In the **Settings** window for **General Form PDE**, locate the **Conservative Flux** section.

3 Specify the Γ vector as

u_flow	x
v_flow	y

To get the correct equation, finish by setting the source and mass terms to zero.

4 Locate the **Source Term** section. In the f text field, type `0`.

5 Locate the **Damping or Mass Coefficient** section. In the d_a text field, type `0`.

Inlet - p=0

1 In the **Physics** toolbar, click **Boundaries** and choose **Dirichlet Boundary Condition**.

As boundary conditions, set pressures at the system's inlet and outlet.

2 In the **Settings** window for **Dirichlet Boundary Condition**, type `Inlet - p=0` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Inlet**.

Outlet - p=p1

1 In the **Physics** toolbar, click **Boundaries** and choose **Dirichlet Boundary Condition**.

2 In the **Settings** window for **Dirichlet Boundary Condition**, type `Outlet - p=p1` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Outlet**.

4 Locate the **Dirichlet Boundary Condition** section. In the r text field, type `p1`.

Last, fill in the mass transport properties of the charged tracer species.

TRANSPORT OF DILUTED SPECIES (TDS)

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

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

3 Select the **Migration in electric field** check box.

Make all necessary interface couplings in the Transport Properties node.

Transport Properties 1

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

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

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

4 Locate the **Diffusion** section. In the D_c text field, type `D`.

5 Locate the **Migration in Electric Field** section. In the z_c text field, type `zn`.

6 Locate the **Convection** section. Specify the $\mathbf{u}$ vector as

u_flow	x
v_flow	y

7 Locate the **Migration in Electric Field** section. From the *V* list, choose **Electric potential (ec)**.

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 *c* text field, type `c_init`.

Set the sum of the convective and diffusive fluxes at the inlet and outlet boundaries to zero with a Flux condition equal to the migration flux (electrophoretic flux=`tds.nmflux_c`).

Flux 1

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

2 Select Boundaries 1 and 10 only.

3 In the **Settings** window for **Flux**, locate the **Inward Flux** section.

4 Select the **Species c** check box.

5 In the $J_{0,c}$ text field, type `-tds.nmflux_c`.

Before solving, improve 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 **Physics-Controlled Mesh** section.

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

Solve the model in two steps: First, compute a stationary (steady-state) solution for the velocity and current density distributions. Then, use this solution to compute the time-dependent tracer concentration distribution.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

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

3 In the table, clear the **Solve for** check box for **Transport of Diluted Species (tds)**.

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent> Time Dependent**.

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

3 In the **Output times** text field, type `range(0,0.1,2)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `0.005`.

6 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check boxes for **Electric Currents (ec)** and **Electroosmotic Pressure (g)**.

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

RESULTS

Concentration (tds)

The surface plot in the third plot group shows the concentration at `t` = 2 s. Under **Results> Export** in the model tree, you can add an Animation node to see how the distribution evolves with time. Alternatively, to reproduce the plot in Figure 3, showing the concentration distribution at four different times, follow the steps below.

Streamline 1

1 In the **Model Builder** window, expand the **Concentration (tds)** node.

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

Surface 1

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

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 From the **Time (s)** list, choose **0**.

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

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

7 In the **Concentration (tds)** toolbar, click **Plot**.

8 Locate the **Data** section. From the **Time (s)** list, choose **0.6**.

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

10 In the **Concentration (tds)** toolbar, click **Plot**.

11 From the **Time (s)** list, choose **1.2**.

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

13 In the **Concentration (tds)** toolbar, click **Plot**.

14 From the **Time (s)** list, choose **1.8**.

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

16 In the **Concentration (tds)** toolbar, click **Plot**.

Proceed to study the effects of each of the two driving forces — the pressure gradient and the electric field — on the velocity field by reproducing the plots in Figure 2. First visualize the velocity field that results from the electric field alone.

Velocity electroosmotic term

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution Store 1 (sol2)**.

Velocity magnitude

1 Right-click **Velocity electroosmotic term** and choose **Surface**.

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

3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>U_eo - Flow-velocity electroosmosis term, magnitude - m/s**.

4 Locate the **Expression** section. From the **Unit** list, choose **mm/s**.

Velocity field

1 In the **Model Builder** window, right-click **Velocity electroosmotic term** and choose **Arrow Surface**.

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

3 Locate the **Expression** section. In the **X component** text field, type `u_eo`.

4 In the **Y component** text field, type `v_eo`.

5 Select the **Description** check box.

6 In the associated text field, type `Velocity electroosmotic term`.

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

8 In the **Velocity electroosmotic term** toolbar, click **Plot**.

Next, plot the velocity field that results from the pressure gradient.

Velocity pressure term

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution Store 1 (sol2)**.

Velocity magnitude

1 Right-click **Velocity pressure term** and choose **Surface**.

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

3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>U_p - Velocity pressure term, magnitude - m/s**.

4 Locate the **Expression** section. From the **Unit** list, choose **mm/s**.

Velocity field

1 In the **Model Builder** window, right-click **Velocity pressure term** and choose **Arrow Surface**.

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

3 Locate the **Expression** section. In the **X component** text field, type `u_p`.

4 In the **Y component** text field, type `v_p`.

5 Select the **Description** check box.

6 In the associated text field, type `Velocity pressure term`.

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

8 In the **Velocity pressure term** toolbar, click **Plot**.

Finally, reproduce the cross-section plot of the concentration along the line $y = 2.5$ mm shown in Figure 4. First define a Cut Line 2D dataset.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

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

3 In row **Point 1**, set **X** to `-4` and **y** to `2.5`.

4 In row **Point 2**, set **X** to `4` and **y** to `2.5`.

Concentration along x-axis @ y=2.5mm

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration along x-axis @ y=2.5mm` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Time selection** list, choose **From list**.

5 In the **Times (s)** list, choose **0**, **0.5**, **1**, **1.5**, and **2**.

Line Graph 1

1 Right-click **Concentration along x-axis @ y=2.5mm** and choose **Line Graph**.

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 Diluted Species>Species c>c - Concentration - mol/m³**.

3 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)>Geometry>Coordinate>x - x-coordinate**.

4 In the **Concentration along x-axis @ y=2.5mm** toolbar, click **Plot**.

Finish by renaming the second plot group.

Pressure

1 In the **Model Builder** window, under **Results** click **2D Plot Group 2**.

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