Transport in an Electrokinetic Valve

This model presents an example of pressure-driven flow and electrophoresis in a microchannel system.

The modeled device is often used as an electrokinetic sample injector in biochips. It is used to get well-defined sample volumes of dissociated acids and salts and to transport these volumes. The model presents a study of a pinched injection cross valve during the focusing, injection, and separation stages. Inspiration for the model was taken from a study by Ermakov et. al. (Ref. 1). Focusing is obtained through pressure-driven flow of the sample and buffer solution, which confines the sample in the focusing channel. When steady state has been reached, the pressure-driven flow is turned off and an electric field is applied along the channels. That field drives the dissociated sample ions in the focusing zone at right angles to the focusing channel and through the injection channel. A clean separation of the sample ions is important, so this model examines different configurations of the electric field in this regard.

This specific case does not account for electroosmosis because the channel surfaces are subjected to a treatment that minimizes the extension of the electric double-layer.

Model Definition

Figure 6-9 shows the domain's geometry. The horizontal channel serves as the focusing channel while the vertical channel is the injection channel.

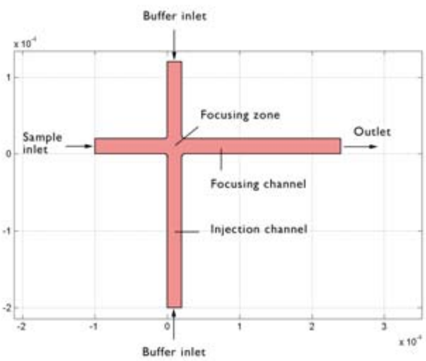


Figure 6-9: The focusing stage involves pressure- and electro-driven flow of the sample and the buffering solution from the left, top, and bottom to the right. An electric field is then applied over the focusing zone to impose transport down through the injection channel.

The focusing stage involves a buffering solution that is injected through pressure-driven convection and electro-driven migration into the vertical channel. The buffering solution neutralizes the acids contained in the sample except for a very thin region confined to the junction between the horizontal and vertical channels. This means that the dissociated ions are found only in the needle-shaped region in the focusing zone.

In the injection stage, convective flow is turned off and an electric field is applied in both the horizontal and vertical directions toward the upper end of the injection channel (see Figure 6-10).

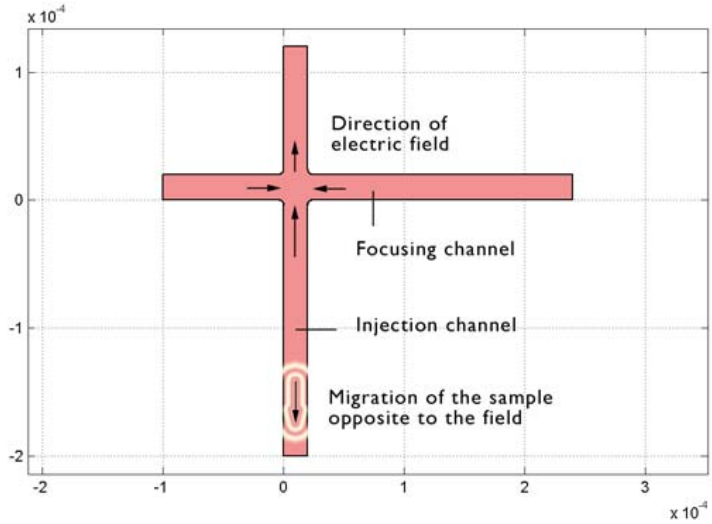


Figure 6-10: During the injection stage, the convective flow is turned off and an electric field is applied. The horizontal field avoids the broadening of the sample while the vertical field injects the sample into the vertical channel in a direction opposite to the electric field.

The horizontal field focuses the sample during the initial part of the injection stage in order to obtain a well-separated sample. The vertical field is applied so as to migrate the sample from the focusing channel to the injection point at the lower end of the vertical channel. The sample ions are negatively charged and migrate in the opposite direction to the electric field. The simulation also covers the case where the horizontal field has not been applied in order to study the effect of sample distortion in the injection stage.

This study assumes that the concentration of charged samples is very low compared to that of other ions dissolved in the solution. This implies that the sample concentration does not influence the solution's conductivity and that you can neglect the concentration gradients of the charge-carrying species, which are present in a much higher concentration than the sample ions. Such an electrolyte is referred to as a supporting electrolyte.

Further assume that concentration variations of the sample species are small in the direction perpendicular to the *x*-*y* plane, which reduces a 3D model to a 2D approximation. This assumption is not entirely true for pressure-driven flow, and a detailed model would treat the third dimension.

The model uses the Navier-Stokes equations, the equation for current balance, and a mass balance based on the Nernst-Planck equation. The steady-state solution for the focusing stage serves as the initial condition for the injection stages.

The boundary conditions are changed between the focusing and injection stages, and the Navier-Stokes equations are not solved during the injection stage because the transport of the charged sample takes place through diffusion and migration (electrophoresis). The model equations are formulated below.

THE FOCUSING STAGE

The Navier-Stokes equations give the global mass a momentum balances in the focusing stage

$$\rho\frac{\partial \mathbf{u}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = 0 \qquad (6\text{-}5)$$
$$\nabla\cdot\mathbf{u} = 0$$

where η denotes the dynamic viscosity (kg/m·s), $\mathbf{u}$ represents the velocity vector (m/s), ρ gives the fluid's density (kg/m^3), and p is the pressure (Pa).

The total balance of charges for a supporting electrolyte is given by the divergence of the current-density vector, which in a supporting electrolyte is given by Ohm's law:

$$\mathbf{i} = -\kappa\nabla\phi \qquad (6\text{-}6)$$

where κ is the electrolyte's conductivity (S/m), and ϕ is the potential (V).

You can now set up a balance of current at steady state

$$\nabla\cdot\mathbf{i} = 0 \qquad (6\text{-}7)$$

which gives

$$\nabla\cdot(-\kappa\nabla\phi) = 0\,. \qquad (6\text{-}8)$$

The flux vector for the sample ions is given by the Nernst-Planck equation

$$\mathbf{N}_i = -D_i\nabla c_i - z_i u_i F c_i\nabla\phi + c_i\mathbf{u}\,, \qquad (6\text{-}9)$$

which for the focusing stage is solved in combination with a mass balance at steady-state for species i:

$$\nabla\cdot(-D_i\nabla c_i - z_i u_i F c_i\nabla\phi + c_i\mathbf{u}) = 0 \qquad (6\text{-}10)$$

where c_i is the concentration (mole/m^3), D_i are the diffusivities (m^2/s), z_i is the charge, u_i represents the mobility (mol ·m^2/J·s), F equals Faraday's constant (A·s/mole), and ϕ is the potential (V).

The boundary conditions for these equations follow. The model solves the Navier-Stokes equations assuming a parabolic profile at the sample and buffer inlet boundaries:

$$\mathbf{u} \cdot \mathbf{n} = v_{mean} 6s(1-s) \tag{6-11}$$

where s denotes a boundary coordinate that goes from 0 to 1 along the respective inlet boundary. This is the Pouseuille equation for fully developed laminar flow in a channel. At the outlet, the velocity component tangential to the boundary is negligible and the pressure is constant. This gives

$$\mathbf{u} \cdot \mathbf{t} = 0 \tag{6-12}$$

and

$$p = 0 \tag{6-13}$$

where p is the relative pressure.

The boundary conditions for the balance of charge determines the potential at the respective inlet and outlet boundary:

$$\phi = \phi_{0,i} \tag{6-14}$$

where i denotes the index for each boundary. All wall boundaries are assumed insulating so that

$$\nabla\phi \cdot \mathbf{n} = 0\,. \tag{6-15}$$

The boundary conditions for the mass balance of the sample during the focusing stage appear next. The first equation gives the concentration at the inlet of the sample, while the second equation gives the concentration of the buffer at the inlet of the two vertical channels:

$$c = c_{\text{in}} \tag{6-16}$$

$$c = c_{\text{buffer}} \tag{6-17}$$

where the buffer inlets are placed at both boundaries in the vertical channel. The outlet boundary states that convection and migration are the dominating transport mechanisms at the outlet (diffusion is negligible). This gives

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_i F c_i \nabla\phi + c_i \mathbf{u}) \cdot \mathbf{n}\,. \tag{6-18}$$

THE INJECTION AND SEPARATION STAGES

In the injection and separation stages, the flow is turned off and the configuration of the electric field is changed. Equation 6-8 is solved again but with new boundary conditions.

The mass balance for the dilute species is given by a time-dependent mass balance

$$\frac{\partial c}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_i F c_i \nabla\phi) = 0 \tag{6-19}$$

where the convective contribution is assumed to be zero.

The boundary conditions for the current-balance equation implies that the potential is locked at all boundaries except for the walls,

$$\phi = \phi_{0,\,i}\,. \tag{6-20}$$

The walls are assumed to be electrically insulated

$$\nabla\phi \cdot \mathbf{n} = 0\,. \tag{6-21}$$

The boundaries for the mass balance are changed compared to the focusing stage. In the injection and separation stages the concentration is set at the inlet boundary according to

$$c = c_{in}\,, \tag{6-22}$$

while all other boundaries are left open, assuming that migration is the dominating transport at the boundaries:

$$\mathbf{N}_i \cdot \mathbf{n} = (-z_i u_i F c_i \nabla\phi) \cdot \mathbf{n}$$

which is an excellent assumption assuming that the sample top has not reached the boundary.

The time-dependent solution requires an initial condition for the mass balance. It is

$$c(t = 0) = c_{focus}$$

where the concentration comes from the steady-state solution obtained from the focusing stage.

Results and Discussion

This study covers two configurations for the potential. In the first configuration—Mode A—the electric field in the injection stage is applied only over the injection channel. Figure 6-11 depicts the resulting concentration distribution in a time sequence.

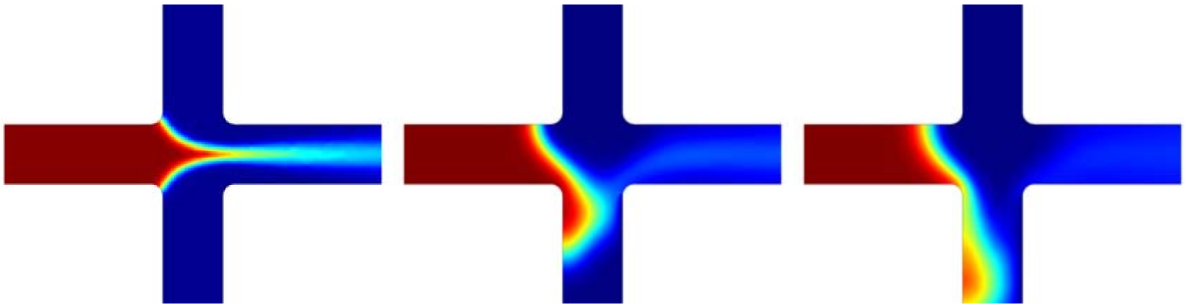


Figure 6-11: The concentration distribution during the focusing (left) and injection stages (middle and right) in the electrokinetic valve's junction where the separation step is part of the injection stage. The graph of the separation step shows that there is incomplete detachment of the sample.

The figure clearly shows that the detachment of the sample during the separation process is incomplete. In fact, if the separated sample is allowed to travel further down the injection channel, the poorly separated region remains attached to the focusing zone. This is also visible in Figure 6-12, which shows the cross section of the concentration profiles at different time steps during the simulation, 5 μm from the left wall of the injection channel. The maximum in concentration moves downwards along the injection channel, but a part of the sample remains attached to the focusing zone.

This effect gives an unwanted distortion of the sample and a deviation from a required bell-curve shape for the concentration profile.

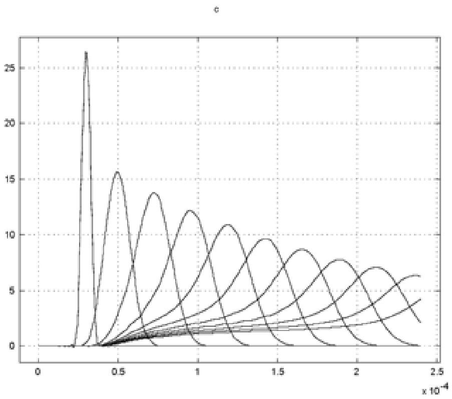


Figure 6-12: Concentration profile along the length of the injection channel at different time steps; 0s, 0.06s, 0.12s, 0.18s, 0.24s, 0.3s, 0.36s, 0.42s, 0.48s, 0.54s, and 0.6s after initiation of the injection stage. The incomplete detachment is clearly seen in the graph.

To avoid broadening of the sample top and to ensure total detachment, an electric field is applied in the horizontal direction, inward from both ends to the focusing zone—Mode B. Now examine results from that simulation:

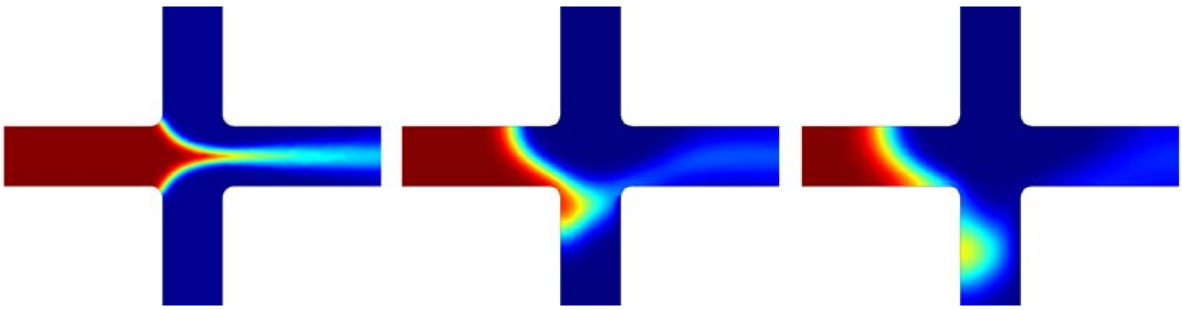


Figure 6-13: In this case the sample has almost completely detached during the separation stage compared to the results in Figure 6-11. It should be mentioned that the electric field strength has a different distribution, which gives a slightly lower migration rate.

Figure 6-13 shows the improved detachment effect that the horizontal field has on the separation of the sample. This is even clearer in Figure 6-14, in which the concentration profile forms a nice bell curve throughout the downward transport in the injection channel.

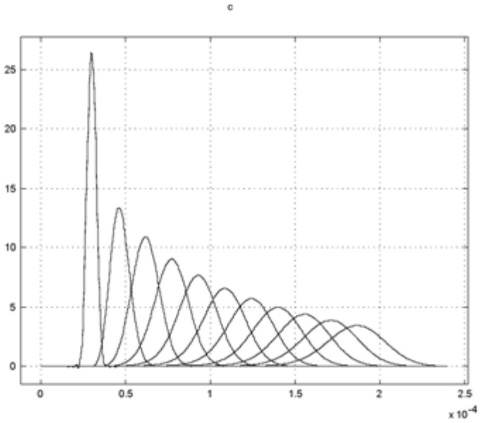


Figure 6-14: Concentration profile along the length of the injection channel at different time steps: 0s, 0.06s, 0.12s, 0.18s, 0.24s, 0.3s, 0.36s, 0.42s, 0.48s, 0.54s, and 0.6s after initiation of the injection stage. The separation of the sample is substantially improved compared to the graphs in Figure 6-12.

This study clearly shows that modeling is extremely valuable in the investigation of electrophoretic transport. You can vary the configuration of the potential to obtain even better focusing and injection stages for the studied valve.

Reference

1. S.V. Ermakov, S.C. Jacobson, and J.M. Ramsey, *Tech. Proc. 1999 Intl. Conf. on Modeling and Simulation of Microsystems*, Computational Publications, 1999.

Modeling in COMSOL Multiphysics

The COMSOL Multiphysics implementation is reasonably straightforward but deserves a few comments. The main strategy is first to solve the equations for the focusing stage using the nonlinear stationary solver and then for the injection stage using both the stationary and time-dependent solvers. The main steps are summarized here:

1 Solve the steady-state problem for the focusing stage, which involves the Navier-Stokes, charge-balance, and mass-balance equations.

2 Store the solution.

3 Change the boundary conditions for the charge balance and re-solve the equation for this balance only. Keep the solution for the concentration field unchanged.
4 Store the solution.
5 Change the boundary conditions for the mass balance.
6 Change the settings to a time-dependent problem and set the velocity components u and v to zero in the Nernst-Planck application mode.
7 Re-solve the problem.

Model Library path:
`Chemical_Engineering_Module/Microfluidics/electrokinetic_valve`

Modeling Using the Graphical User Interface

1 In the **Model Navigator** set the **Space dimension** to **2D**.
2 In the list of application modes select
Chemical Engineering Module>Momentum Balance>Incompressible Navier-Stokes.
3 Click the **Multiphysics** button, then click **Add**.
4 Similarly add two more application modes:
Chemical Engineering Module>Mass Balance>Electrokinetic flow
COMSOL Multiphysics>Electromagnetics>Conductive Media DC.
5 Click **OK**.

OPTIONS AND SETTINGS

1 Select **Constants** from the **Options** menu.
2 Add the constants in the following table; when done, click **OK**:

NAME	EXPRESSION
u_max	3e-4
v_max	1e-3
rho	1e3
eta	1e-3
D	2e-10
mob	1e-9/8.31/298
c_in	3.5/(22/35)*1e3*5e-3

GEOMETRY MODELING

1 Hold the shift key and click the **Rectangle/Square** button on the Draw toolbar.

2 In the **Rectangle** dialog box that appears, enter these properties; when done, click **OK**:

PARAMETER	VALUE
Width	`2e-5`
Height	`3.2e-4`
x position	`0`
y position	`-2e-4`

3 Repeat this procedure for one more rectangle with these dimensions; when done, click **OK**:

PARAMETER	VALUE
Width	`3.4e-4`
Height	`2e-5`
x position	`-1e-4`
y position	`0`

4 Click the **Zoom Extents** button on the Main toolbar.

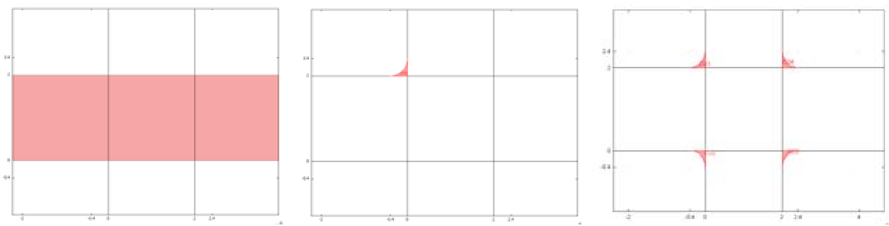
5 Select **Axes/Grid Settings** from the **Options** menu.

6 Click the **Grid** tab, clear the **Auto** check box, and enter `2e-5` in both the **x spacing** and **y spacing** edit fields.

7 Type `-4e-6 2.4e-5` in the **Extra x** edit field and `-4e-6 2.4e-5` in the **Extra y** field.

8 Click **OK**.

9 Click the **Zoom Window** button on the Main toolbar and zoom in on the junction area.



10 Select the **2nd Degree Bezier Curve** tool on the Draw toolbar and click on the points (-4e-6, 2e-5), (0, 2e-5), and (0, 2.4e-5).

11 Click the **Line** button and click on the corner (0, 2e-5).

12 Click the right mouse button to create a solid composite object.

13 In a similar fashion, create smoothed corners for the three other corners.

14 Press Ctrl+A to select all the geometry objects.

15 Click the **Union** button on the Draw toolbar and finally the **Delete interior boundaries** button on the Draw toolbar.

PHYSICS SETTINGS—FOCUSING STAGE

Boundary Conditions

1 Select **1 Incompressible Navier-Stokes (chns)** from the **Multiphysics** menu.

2 Select **Boundary Settings** from the **Physics** menu.

3 Specify the conditions in the following table; when done, click **OK**:

BOUNDARY	1	2–4, 6, 8–11, 13–16	5	7	12
Boundary condition	Inflow/Outflow velocity	No-slip	Inflow/Outflow velocity	Inflow/Outflow velocity	Normal flow/ Pressure
u_0	`u_max*4*s*(1-s)`		0	0	
v_0	0		`v_max*4*s*(1-s)`	`-v_max*4*s*(1-s)`	
p_0	-	-	-	-	0

4 Select **2 Electrokinetic Flow (chekf)** from the **Multiphysics** menu

5 Set the boundary conditions as in the following table; when done, click **OK**:

BOUNDARY	1	2-4, 6, 8-11, 13-16	5, 7	12
Boundary condition	Concentration	Insulation/ symmetry	Concentration	Convective flux
c_0	`c_in`		0	

6 Select **3 Conductive Media DC (dc)** from the **Multiphysics** menu

7 Set the boundary conditions as the following table; when done, click **OK**:

BOUNDARY	1	2-11, 13-16	12
Boundary condition	Electric potential	Electric insulation	Ground
V_0	-1		

Subdomain Settings

1 From the **Multiphysics** menu select **1 Incompressible Navier-Stokes (chns)**.

2 Open the **Subdomain Settings** dialog box from the **Physics** menu.

3 Enter these subdomain conditions; when done, click **OK**:

SUBDOMAIN	1
ρ	`rho`
η	`eta`
F_x	0
F_y	0

4 Select **2 Electrokinetic Flow (chekf)** from the **Multiphysics** menu.

5 Enter these subdomain settings; when done, click **OK**:

SUBDOMAIN	1
D (isotropic)	`D`
R	0
u_m	`mob`
z	-1
u	`u`
v	`v`
V	`V`

6 Select **3 Conductive Media DC (dc)** from the **Multiphysics** menu.

7 Enter these subdomain settings; when done, click **OK**:

SUBDOMAIN	1
σ (isotropic)	1
Q_j	0
$\mathbf{J}^e$	[0 0]

MESH GENERATION

1 Select **Free Mesh Parameters** from the **Mesh** menu.

2 Click the **Custom mesh size** button and change the **Mesh curvature factor** to `0.6`.

3 Type `1e-5` in the **Maximum element size** edit field.

4 Click **Remesh**, then click **OK**.

COMPUTING THE SOLUTION—FOCUSING STAGE

Start by computing the solution for the velocity field and then use that solution when solving the mass-transport problem.

1 Click the **Solver Manager** button on the Main toolbar.
2 Click the **Solve For** tab and select **Incompressible Navier-Stokes (chns)**.
3 Click the **Initial Value** tab and click the **Initial value expression** option.
4 Click **OK**.
5 Open the **Solver Parameters** dialog box from the **Solve** menu.
6 Select **Stationary nonlinear** from the **Solver** list. Click **OK**.
7 Click the **Solve** button on the Main toolbar.
8 When the solver has completed, open the **Solver Manager** dialog box to the **Solve For** page and switch to **Conductive Media DC**.
9 Click **OK** and click the **Restart** button on the Main toolbar.
10 Open the **Solver Manager** dialog box to the **Solve For** page and switch to **Electrokinetic flow**.
11 Click **OK** and click the **Restart** button on the Main toolbar.

The focusing stage is now complete. In the next step you solve the model for the transient problem that describes the injection and separation stages.

PHYSICS SETTINGS—INJECTION STAGE, MODE A

Boundary Conditions

1 Change the boundary settings for the **Conductive Media DC** application mode as follows; when done, click **OK**:

BOUNDARY	1	5	7	12	ALL OTHERS
Boundary condition	Electric insulation	Electric potential	Electric potential	Electric insulation	Electric insulation
V_0	-	0	-3.2	-	-

2 Change the boundary settings for the **Electrokinetic flow** mode as follows; when done, click **OK**:

BOUNDARY	1	5	7	12	ALL OTHERS
Boundary condition	Flux	Flux	Flux	Flux	Convective Flux
N_0	F_chekf*mob*c*Vx	F_chekf*mob*c*Vy	-F_chekf*mob*c*Vy	-F_chekf*mob*c*Vx	-

Subdomain Settings

In the **Subdomain Settings** dialog box for the **Electrokinetic flow** mode, change **u** and **v** to `0`. Click **OK**.

COMPUTING THE SOLUTION—INJECTION STAGE, MODE A

1. Click the **Solver Manager** button on the Main toolbar.
2. Click the **Initial Value** tab, click the **Store Solution** button, and click the **Stored solution** option in the **Initial value** area.
3. Click the **Solve For** tab and select **Conductive Media (dc)**. Click **OK**.
4. Click the **Solve** button on the Main toolbar.
5. From the **Solve** menu open the **Solver Manager** dialog box.
6. Click the **Store Solution** button on the **Initial Value** page.
7. On the **Solve For** page select only **Electrokinetic flow**.
8. Open the **Solver Parameters** dialog box from the **Solve** menu.
9. Select **Time dependent** from the **Solver** list.
10. Type `0:0.03:0.6` in the **Times** edit field.
11. Click **OK**.
12. On the Main toolbar click the **Solve** button.

POSTPROCESSING AND VISUALIZATION—MODE A

To create Figure 6-11 on page 280, follow these steps:

1. From the **Options** menu open the **Axes/Grid settings** dialog box.
2. On the **Grid** page select the **Auto** check box.
3. On the **Axis** page set **x min** = **y min** = `-4e-5` and **x max** = **y max** = `6e-5`. Click **OK**.
4. From the **Postprocessing** menu open the **Plot Parameters** dialog box.
5. On the **General** page clear the **Element refinement Auto** check box and type `5` in the corresponding edit field.
6. Select **0** from the **Solution at time** list.
7. Select the **Surface** tab and set **Surface data** and choose **Concentration, c** from the **Predefined quantities** list.
8. Click **Apply**.
9. Select the **General** tab and select **0.06** from the **Solution at time** list. Click **Apply**.
10. Select **0.12** from the **Solution at time** list. Click **OK**.

Figure 6-12 is created with the cross-section plot function.

1 Select **Cross-Section Plot Parameters** from the **Postprocessing** menu.
2 On the **General** page select every other time step from the **Solutions to use** list.
3 Click the **Line/Extrusion** tab.
4 Set **y-axis data** to **Concentration, c (chekf)**.
5 Under **Cross-section line data**, set these parameters:

PROPERTY	VALUE
x0	0.1e-4
x1	0.1e-4
y0	0.4e-4
y1	-2e-4

6 Click the **Line Settings** button.
7 Select **Color** from the **Line color** list.
8 Click the **Color** button and specify the color as black. Click **OK** three times.

PHYSICS SETTINGS—INJECTION STAGE, MODE B

The next step is to model the second configuration of the electric field—Mode B.

Boundary Conditions

Change the boundary settings for the **Conductive Media DC** application mode as follows; when done, click **OK**:

BOUNDARY	1	5	7	12	ALL OTHERS
Boundary condition	Electric potential	Electric potential	Electric potential	Electric potential	Electric insulation
V_0	-1	0	-3.2	0	-

COMPUTING THE SOLUTION—INJECTION STAGE, MODE B

1 Click the **Solver Manager** button on the Main toolbar.
2 On the **Solve For** page select **Conductive Media DC (dc)**, then click **OK**.
3 in the **Solve>Solver Parameters** dialog box select the **Stationary** solver.
4 Click the **Solve** button on the Main toolbar.
5 In the **Solver Manager** dialog box click the **Store Solution** button on the **Initial Value** page.

6 On the **Solve For** page select only **Electrokinetic flow**.

7 Open the **Solver Parameters** dialog box from the **Solve** menu.

8 Select **Time dependent** from the **Solver** list.

9 Click **OK** and then click **Solve**.

POSTPROCESSING AND VISUALIZATION—MODE B

You create the figures for Mode B in exactly the same way as the figures for Mode A.