

COMSOL MULTIPHYSICS™

AC Electrokinetically Enhanced Surface Reactions

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AC Electrokinetically Enhanced Surface Reactions

Introduction

This model studies the use of AC electrokinetic forces to enhance the rate of transport of reactants to a reaction surface on the wall of a microchannel. It was developed for the MEMS Module by Gaurav Soni, Marin Sigurdson, and Carl Meinhart of the Department of Mechanical and Environmental Engineering, University of California, Santa Barbara.

The modeled system mixes a small concentration of a biological analyte with the fluid in a microchannel where a reaction surface is located on the channel walls. The flow velocity perpendicular to the surface is so small that the analyte, which is supposed to bind to an antibody ligand on this surface, is transported mainly by diffusion. The rate of the binding reaction on the surface is usually large enough to bind practically all analyte molecules appearing there. Thus, the process is said to be transport limited and, in order to increase the reaction rate, the system must increase the transport of molecules to the reaction surface.

AC electrokinetic forces can generate swirling patterns in the fluid and thereby enhance the transport of the analyte to the reaction surface (Ref. 1). Biological immunoassays, which detect an analyte through their binding response to an antibody ligand, can use these flow patterns to great advantage.

The AC electrokinetic forces arise when the fluid absorbs energy from an applied nonuniform AC electric field by means of Joule heating. The temperature increase changes the fluid's conductivity and permittivity. Consequently the fluid experiences an effective or time-averaged volume force, which depends on the conductivity and permittivity gradients and on the field intensity. By changing the shape of the electric field it is possible to alter the fluid-flow pattern so that required amounts of analyte molecules reach the reaction surface.

Model Definition

Figure 1 shows the model geometry, which consists of a section of the channel 40 μm high and 250 μm long. Two electrodes, each 60 μm wide, are located on the lower

boundary at distances of 50 μm and 130 μm from the inlet. The reaction surface, 20 μm wide, is located on the top wall, 90 μm from the inlet.

The fluid flows from left to right. The incoming flow profile is characteristic for fully developed laminar flow, that is, it is parabolic with zero velocity at the channel walls. An applied electrothermal force creates swirling patterns in the flow at the channel's center.

The two electrodes produce an AC electric field that heats the fluid and creates the electrothermal force. The model assumes that the electrodes are perfect heat conductors and remain at a constant ambient temperature. At the inlet and the outlet, the temperature gradually approaches the ambient. At all other boundaries the model assumes that the channel is thermally and electrically insulated.

The incoming flow has a small concentration of a biological analyte, which the reaction surface on the upper boundary transports and adsorbs. Any remaining concentration exits the channel with the fluid at the right boundary.

Having solved for the steady-state flow for a given electric field and the resulting electrothermal force, this example reviews a transient simulation of the material balance of the analyte, assuming that the initial concentration in the channel is zero and that a given concentration of the analyte is injected at the inlet at time zero.

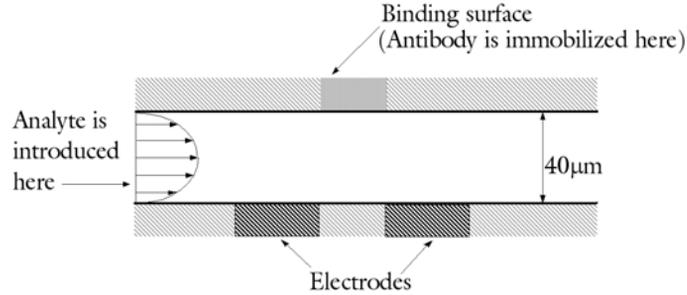


Figure 1: Model geometry for the microchannel with electrodes and a reaction surface.

FLUID FLOW

Fluid flow in the channel follows the Navier-Stokes equations

$$\rho \frac{\partial \mathbf{u}}{\partial t} - \eta \nabla^2 \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{F}$$

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

where \mathbf{u} denotes the velocity, ρ is the density, η is the dynamic viscosity, and p refers to the pressure. At steady state, the first time-dependent term disappears. The volume force \mathbf{F} appearing in the equation is the electrothermal force \mathbf{f}_E given by

$$\mathbf{F} = \mathbf{f}_E \quad (1)$$

$$\mathbf{f}_E = -0.5 \left[\left(\frac{\nabla \sigma}{\sigma} + \frac{\nabla \epsilon}{\epsilon} \right) \cdot \mathbf{E} \frac{\epsilon \mathbf{E}}{1 + (\omega \tau)^2} + 0.5 |\mathbf{E}|^2 \nabla \epsilon \right]$$

where σ is the conductivity, $\epsilon = \epsilon_r \epsilon_0$ equals the fluid's permittivity, ω represents the electric field's angular frequency, and $\tau = \epsilon / \sigma$ gives the fluid's charge-relaxation time. The field vector \mathbf{E} contains the amplitude and orientation of the AC electric field but not its instantaneous value.

The following table gives the input data for the model:

NAME	VALUE	DESCRIPTION
ρ	1000 kg/m ³	Density of water
η	1.08 · 10 ⁻³ kg/(m·s)	Dynamic viscosity of water
σ	5.75 · 10 ⁻² S/m	Conductivity of water
ϵ_r	80.2	Relative permittivity of water
ω	2π · 15 · 10 ³ rad/s	Angular frequency of the AC electric field

As a result of Joule heating, ϵ and σ are temperature dependent. You can rewrite the gradients of these entities using chain differentiation, which yields

$$\nabla \epsilon = (\partial \epsilon / \partial T) \nabla T$$

and

$$\nabla \sigma = (\partial \sigma / \partial T) \nabla T$$

where T is the fluid's temperature. For water,

$$(1/\epsilon)(\partial \epsilon / \partial T) = -0.004 \text{ K}^{-1}$$

and

$$(1/\sigma)(\partial \sigma / \partial T) = 0.02 \text{ K}^{-1}$$

Thus you can rewrite the electrothermal force (Equation 1) as

$$\mathbf{f}_E = -0.5\epsilon \left((0.016 \text{ K}^{-1}) \nabla T \cdot \mathbf{E} \frac{\mathbf{E}}{1 + (\omega\tau)^2} + 0.5|\mathbf{E}|^2 (-0.004 \text{ K}^{-1}) \nabla T \right)$$

The following table contains the boundary conditions for the incompressible Navier-Stokes equations:

BOUNDARY	CONDITION
Left	Parabolic inflow with average velocity 0.1 mm/s and zero velocity at the upper and lower boundaries
Upper	No slip condition
Lower	No slip condition
Right	Outflow with pressure $p = 0$

ELECTROSTATICS

Because the electrothermal force is a time-averaged entity, it is sufficient to solve the static electric field that corresponds to the root mean square (rms) value of the AC field. The rms value of the AC voltage is $V_{\text{rms}} = 10 \text{ V}$.

To solve the electrostatics problem, turn to Laplace's equation

$$-\nabla \cdot (\epsilon \nabla V) = 0$$

with

$$\mathbf{E} = -\nabla V$$

and the constitutive equation

$$\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$$

The boundary conditions for the electrostatic problem are as follows:

BOUNDARY	CONDITION
Left electrode	Electric potential, $V = V_{\text{rms}}/2 = 5\text{V}$
Right electrode	Electric potential, $V = -V_{\text{rms}}/2 = -5\text{V}$
Other boundaries	Electric insulation

HEAT TRANSFER

The power that a unit volume of fluid absorbs through Joule heating is

$$Q = \sigma |\mathbf{E}|^2$$

where \mathbf{E} is the rms value of the electric field and σ is the fluid's conductivity. The heat source, Q , appears in the stationary heat balance equation

$$\nabla \cdot (-k\nabla T) = Q - \rho C_p \mathbf{u} \cdot \nabla T$$

where C_p denotes the heat capacity and k is the fluid's thermal conductivity. This is the nonconservative formulation of the heat balance, which is consistent with the assumption of a divergence-free flow field.

The following table gives the relevant input data for the heat-transfer problem:

NAME	VALUE	DESCRIPTION
ρ	1000 kg/m ³	Density of water
C_p	4.184 · 10 ³ J/(kg·K)	Heat capacity of water
k	0.598 W/(m·K)	Thermal conductivity of water

In general, the Navier-Stokes equations along with the convection and conduction equation form a coupled system that you should solve simultaneously.

This example assumes an ambient temperature $T = 0$ °C, and the electrodes are held steady at this temperature. The flow rate is small, and you can therefore assume that the temperature decreases symmetrically at the inlet and the outlet. The magnitude of the temperature gradient at both boundaries is such that the fluid reaches the ambient temperature at a distance of 1 mm from the boundary. At all other boundaries the model assumes that the channel is insulated.

CONVECTION AND DIFFUSION OF THE ANALYTE

The material balance of the analyte comes from the equation

$$\delta_{ts} \frac{\partial c}{\partial t} + \nabla \cdot (-D\nabla c) = R - \mathbf{u} \cdot \nabla c .$$

This equation gives the material balance in a nonconservative form because the flow field is divergence free. In this equation D denotes the diffusion coefficient and R represents the reaction rate. Here R equals zero because no reactions take place in the bulk of the fluid, only on the reaction surface.

The boundary conditions are as follows:

BOUNDARY	CONDITION
Left	The incoming flow has constant analyte concentration
Right	Remaining concentration leaves the system through convection

BOUNDARY	CONDITION
Reaction surface	Concentration consumed in the binding reaction as defined by Equation 2 (see next chapter)
Other boundaries	Boundaries are insulated and the concentration gradients normal to these boundaries equal zero

The following table gives the input data for the material balance:

NAME	VALUE	DESCRIPTION
δ_{ts}	1	Time-scaling coefficient
D	$1 \cdot 10^{-11} \text{ m}^2/\text{s}$	Diffusivity of the analyte in the fluid
R	0 M/s	No reaction takes place within the fluid
c_0	1 nM = $1 \mu\text{mol}/\text{m}^3$	Inlet analyte concentration

BINDING REACTION

The reaction surface contains a total concentration R_t of antibody ligands. The portion of the bonded molecules is the concentration B . The binding rate depends on the analyte concentration on the surface, c , on the concentration of free antibodies, and on the association rate constant, k_{on} . Similarly, bonded antibodies dissociate with a rate that depends on the concentration of the bonded ligands and on the dissociation rate constant, k_{off} . Therefore, the equation that describes the material balance of adsorbed species (see Ref. 2) is:

$$\frac{\partial B}{\partial t} = k_{\text{on}}c(R_t - B) - k_{\text{off}}B \quad (2)$$

The reaction rate of the analyte on the surface equals the negative of the binding rate on the surface.

The table below gives the input data for the material balance of the adsorbed species:

NAME	VALUE	DESCRIPTION
k_{on}	$10^8 (\text{M}\cdot\text{s})^{-1} = 10^5 \text{ m}^3/(\text{mol}\cdot\text{s})$	Association rate constant
k_{off}	0.02 s^{-1}	Dissociation rate constant
R_t	$1.67 \cdot 10^{-11} \text{ M}\cdot\text{m} = 1.67 \cdot 10^{-8} \text{ mol}/\text{m}^2$	Total surface concentration of the antibody ligand

The model assumes that the antibodies do not diffuse on the surface and that there is no leakage of the molecules at the edges of the surface.

To study the effect of the applied electric field, you first run the model with $V_{\text{rms}} = 0$ V and then repeat the simulation for $V_{\text{rms}} = 10$ V.

STEP-RESPONSE ANALYSIS

Another interesting aspect to analyze is the system's behavior when injecting a fixed amount of analyte over a limited time with a sudden cutoff in the analyte supply. To simulate such an experiment, use the analyte inlet concentration expression

$$c(t) = \begin{cases} c_0 & t < t_1 \\ 0 & t > t_1 \end{cases} \quad (3)$$

with $t_1 = 1000$ s and $c_0 = 75$ nM = $75 \mu\text{mol}/\text{m}^3$ ($1 \text{ M} \equiv 1 \text{ mol}/\text{l} = 10^3 \text{ mol}/\text{m}^3$). For this analysis, modify the material balance input data according to the following table to obtain a reaction-rate limited process.

NAME	VALUE	DESCRIPTION
k_{on}	$100 \text{ m}^3/(\text{mol}\cdot\text{s})$	Association rate constant
k_{off}	$5 \cdot 10^{-3} \text{ s}^{-1}$	Dissociation rate constant
R_t	$1.67 \cdot 10^{-11} \text{ mol}/\text{m}^2$	Total surface concentration of the antibody ligand

Results and Discussion

Figure 2 shows the flow profile and concentration distribution without any applied electric field. In this case, the flow is laminar and has a parabolic profile. The effect of the reaction surface on the analyte concentration is visible only in the narrow region near the surface. Compare it to the flow and concentration with an applied electric field (Figure 3). Now the flow profile is far from parabolic: it has two distinct swirls and a narrow region with high flow velocity between the electrodes. Both of these figures represent the situation 5 s after the system introduces analyte at the left boundary.

Figure 4 depicts the flow and concentration just 1 s after introducing the analyte. It shows more clearly how the swirling patterns in the flow focus the analyte on a narrower path near the reaction surface. This flow results in a difference in the adsorption rate of the molecules with and without the electric field, (Figure 5). The average number of adsorbed molecules—the ratio between the total amount and the surface width—on the surface increases more rapidly with the electric field (the curve with squares) than without the electric field (the curve with triangles).

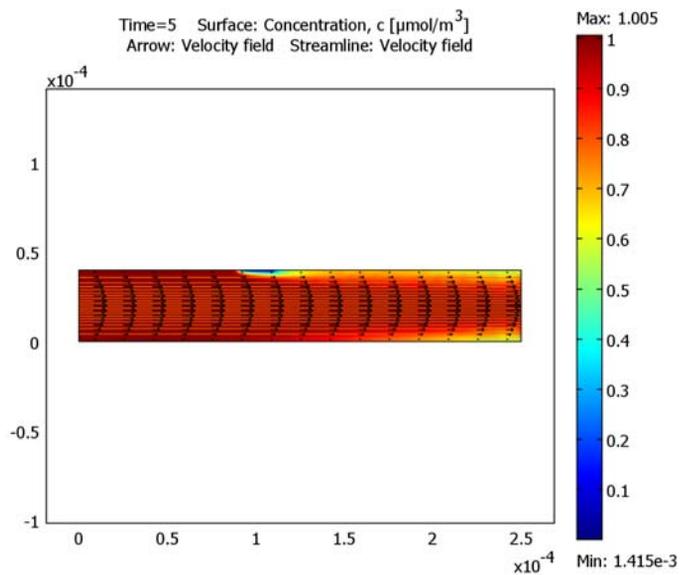


Figure 2: Microchannel flow and concentration at 5 s without any applied electric field.

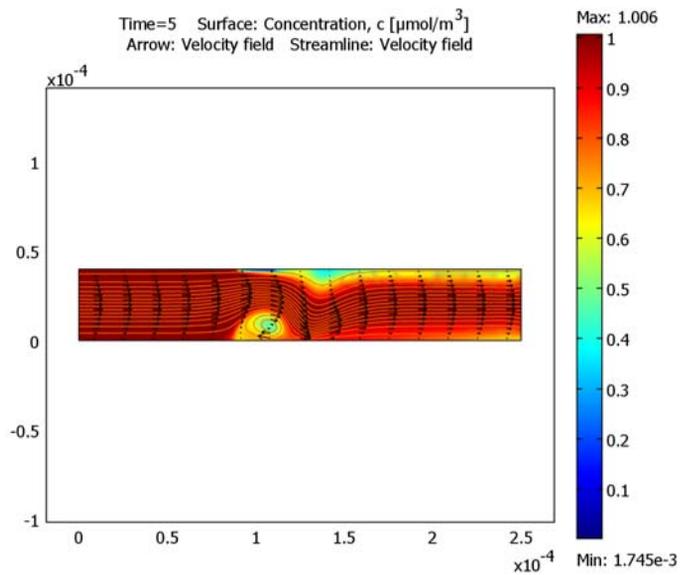


Figure 3: Microchannel flow and concentration at 5 s with an applied electric field.

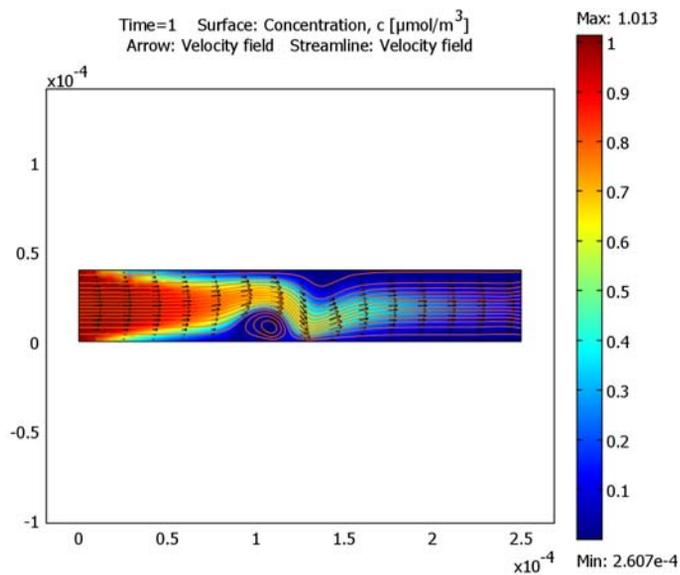


Figure 4: Microchannel flow and concentration at 1 s with an applied electric field.

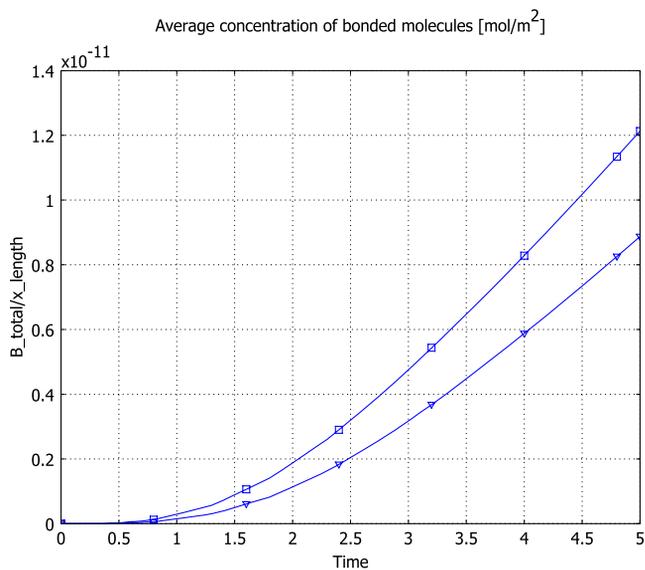


Figure 5: Binding of molecules on the reaction surface in the microchannel with (squares) and without (triangles) an applied electric field.

Figure 6 shows the result for the average concentration of bonded molecules of the third and final simulation, in which you cut off the analyte supply at $t = 1000$ s. During the phase when the analyte supply is kept constant, the concentration of molecules on the binding surface approaches a constant maximum value near 10^{-11} mol/m². When the supply at the inlet then stops, the concentration starts to decay. By varying the antibody ligand concentration and the association and dissociation rate constants, you can study the effects on the maximum concentration and the decay rate. Simulations of this kind can thus be useful for fitting a model to experimental data.

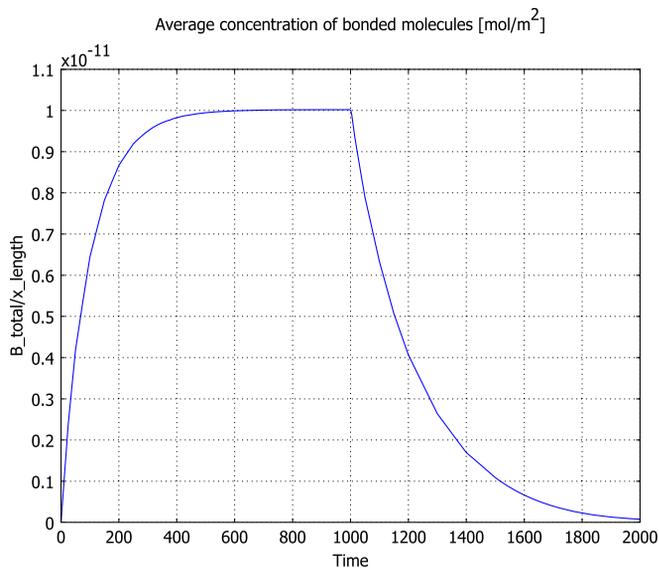


Figure 6: System response when the analyte supply at the inlet is cut off at $t = 1000$ s.

Modeling in COMSOL Multiphysics

This model solves the problem with two geometries and five application modes. Table 1 lists the geometries and their application modes.

The first geometry, named *channel*, is in 2D and represents the channel. Within this geometry the model uses four application modes: Electrostatics, Convection and Conduction, Incompressible Navier-Stokes, and Convection and Diffusion. The second geometry, named *surface*, is in 1D and simulates the reaction surface with the Diffusion application mode. The overall model couples this solution with the reaction

surface boundary condition of the Convection and Diffusion application mode on the first geometry. For this purpose you must define two extrusion-coupling variables.

You solve the model in three steps with different solvers in a progression using results from the previous step:

- First, solve the Electrostatics application mode with a stationary linear solver.
- Next, solve the Convection and Conduction and the Incompressible Navier-Stokes application modes together using a stationary nonlinear solver, because they form a coupled system through their subdomain settings.
- In the third step you use the time-dependent solver to solve the transport of the analyte. At this point the software solves two application modes simultaneously: Convection and Diffusion, and Diffusion.

COMSOL Multiphysics' solver scripting capabilities allow you to record these solving stages, a feature which greatly facilitates repeated simulations.

TABLE 1: GEOMETRY AND APPLICATION MODE DESCRIPTION

GEOMETRY	APPLICATION MODE	VARIABLES	DESCRIPTION
channel	Electrostatics	V	Solves the static electric potential in the channel
channel	Convection and Conduction	T	Solves the temperature distribution in the channel
channel	Incompressible Navier-Stokes	u, v, p	Solves the velocities in the x and y directions and the pressure distribution in the channel
channel	Convection and Diffusion	c	Solves the concentration of the analyte in the channel
surface	Diffusion	B	Solves the concentration of the binded antibodies on the reaction surface

References

1. A. Ramos, H. Morgan, N.G. Green, and A. Castellanos, "AC electrokinetics: A review of forces in microelectrode structures," *J. Phys. D: Appl. Phys.*, vol. 31, pp. 2338–2353, 1998.
2. D.G. Myszka, "Survey of the 1998 optical biosensor literature," *J. Mol. Recognit.*, vol. 12, pp. 390–408, 1999.

Model Library path: MEMS_Module/Microfluidics_Models/
ac_electrokinetic_2d

Modeling Using the Graphical User Interface

MODEL LIBRARY

- 1 In the **Model Navigator**, click the **New** tab, then click the **Multiphysics** button.
- 2 Click the **Add Geometry** button.
- 3 Enter these settings in the dialog box:

FIELD	VALUE
Geometry name	channel
Space dimension	2D
Independent variables	x y z

- 4 Click **OK**.
- 5 Click the **Add Geometry** button once again and enter these settings:

FIELD	VALUE
Geometry name	surface
Space dimension	1D
Independent variables	x y z
Unit system	None

Because the available unit systems give the wrong reference dimension for the 1D geometry, use the last setting to disable units for this geometry.

- 6 Click **OK**.
- 7 In the **Multiphysics** area, select the geometry **channel (2D)**.
- 8 In the list of application modes, select **MEMS Module>Electrostatics>Electrostatics**, then click the **Add** button in the **Multiphysics** area.
- 9 Select the application mode **COMSOL Multiphysics>Heat Transfer>Convection and Conduction**, then click the **Add** button.
- 10 Select **MEMS Module>Microfluidics>Incompressible Navier-Stokes**, then click **Add**.

11 Select **MEMS Module>Microfluidics>Convection and Diffusion>Transient analysis**, then click **Add**.

12 In the **Multiphysics** area, select the geometry **surface (1D)**.

13 Select **COMSOL Multiphysics>Convection and Diffusion>Diffusion>Transient analysis**. In the **Dependent variables** edit field type B, then click **Add**.

14 Click **OK**.

OPTIONS AND SETTINGS

1 From the **Options** menu, choose **Constants**.

2 Define the following names, expressions, and (optionally) descriptions; when finished, click **OK**.

NAME	EXPRESSION	DESCRIPTION
epsilon0	8.854188e-12[F/m]	Permittivity of free space
epsilon_r_f	80.2	Relative permittivity, fluid
epsilon_f	epsilon_r_f*epsilon0	Permittivity, fluid
k_f	0.598[W/(m*K)]	Thermal conductivity, fluid
rho_f	1000[kg/m^3]	Density, fluid
Cp_f	4.184[kJ/(kg*K)]	Heat capacity, fluid
eta_f	1.08e-3[Pa*s]	Dynamic viscosity, fluid
sigma_f	5.75e-2[S/m]	Electric conductivity, fluid
tau	epsilon_f/sigma_f	Charge relaxation time, fluid
D_a	1e-11[m^2/s]	Diffusion coefficient, analyte
omega	2*pi[rad]*15[kHz]	Angular frequency, AC electric field
V_rms	0[V]	Electric potential, RMS value
T_amb	0[degC]	Ambient temperature
u_av	0.1[mm/s]	Average flow velocity at the inlet
c0	1[umol/m^3]	Analyte concentration at the inlet
k_on	1e5[m^3/(mol*s)]	Association rate constant
k_off	0.02[1/s]	Dissociation constant
R_t	1.67e-8[mol/m^2]	Total surface concentration, antibody ligand

Later, you change the value of the electric potential to 10 V and re-solve the model.

GEOMETRY MODELING

First create the 2D geometry for the channel.

- 1 Click the **channel** tab in the drawing area.
- 2 From the **Options** menu, choose **Axes/Grid Settings**.
- 3 In the dialog box, click the **Axis** tab, select the **Axes equal** check box, and enter these settings:

SETTING	VALUE
x min	-5e-5
x max	30e-5
y min	-5e-5
y max	10e-5

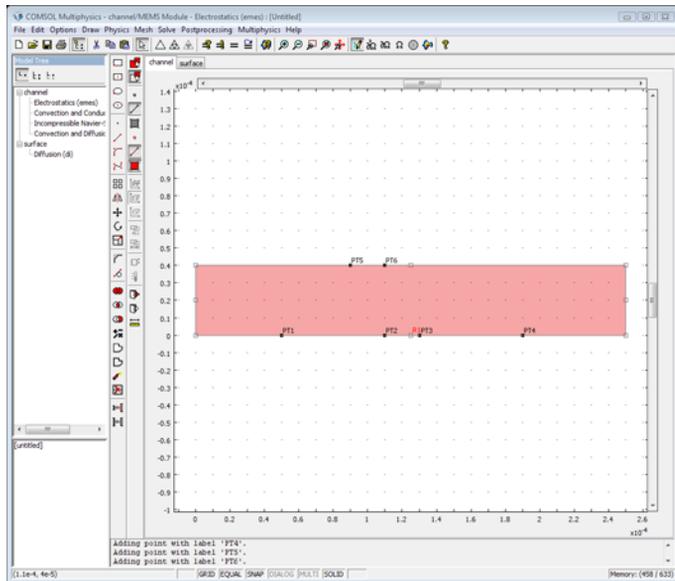
- 4 Click the **Grid** tab.
- 5 Clear the **Auto** check box and make these settings:

SETTING	VALUE
x spacing	1e-5
y spacing	1e-5

- 6 Click **OK**.
- 7 Click the **Rectangle/Square** button on the Draw toolbar and draw a rectangle with diagonally opposite corners at (0, 0) and ($2.5 \cdot 10^{-4}$, $4 \cdot 10^{-5}$).
- 8 Draw the following points by successively using the **Point** tool in the Draw toolbar.

NAME	x	y
PT1	0.5e-4	0
PT2	1.1e-4	0
PT3	1.3e-4	0
PT4	1.9e-4	0
PT5	0.9e-4	0.4e-4
PT6	1.1e-4	0.4e-4

The completed 2D geometry should look like that in the following picture:



The completed 2D geometry for a microchannel detector.

Next create the 1D geometry for the reaction surface.

- 1 Click the **surface** tab.
- 2 From the **Options** menu, choose **Axes/Grid Settings**.
- 3 In the dialog box, click the **Axis** tab, then enter these settings:

SETTING	VALUE
x min	-5e-5
x max	30e-5

- 4 Click the **Grid** tab. Clear the **Auto** check box. In the **x spacing** edit field type $1e-5$, then click **OK**.
 - 5 On the Draw toolbar select the **Line** tool and draw a line from $0.9 \cdot 10^{-4}$ to $1.1 \cdot 10^{-4}$.
- The geometry is now complete.

PHYSICS SETTINGS

Expressions and Coupling Variables

Follow these steps to create the expressions for computing the electrothermal force, to define the expressions and coupling variables needed to solve the binding reaction, and provide the integration-coupling variables needed for postprocessing.

Note: You create expressions separately for the two geometries.

Start by defining scalar expressions for the electrothermal force components.

- 1 Click the **channel** tab to select that geometry.
- 2 From the **Options** menu, choose **Expressions>Scalar Expressions**.
- 3 In the dialog box, enter the expressions in the following table for the x - and y -components of the electrothermal force. Note that this example uses the expressions tmp1 and tmp2 only to simplify the writing of Fx_et and Fy_et.

NAME	EXPRESSION
tmp1	$(Tx*Ex_emes+Ty*Ey_emes)/(1+(\omega*\tau)^2)$
tmp2	$normE_emes^2$
Fx_et	$-0.5*\epsilon_f*(0.016[1/K]*tmp1*Ex_emes-0.5*0.004[1/K]*tmp2*T_x)$
Fy_et	$-0.5*\epsilon_f*(0.016[1/K]*tmp1*Ey_emes-0.5*0.004[1/K]*tmp2*T_y)$

- 4 Click **OK**.

Next set the expressions and extrusion-coupling variables you need to solve the surface reaction.

- 1 From the **Options** menu, choose **Expressions>Boundary Expressions**.
- 2 In the **Boundary selection** list, select Boundary 5.
- 3 Create the following boundary expression (c_surf is an extrusion coupling variable that you define later):

NAME	EXPRESSION
react_bulk	$k_off*c_surf-k_on*c*(R_t-c_surf)$

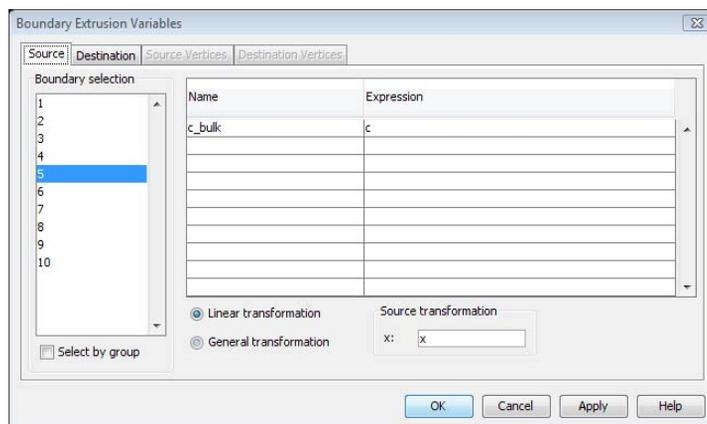
COMSOL Multiphysics marks the unit of react_bulk as inconsistent because of the coupling variable. You can disregard this warning.

- 4 Click **OK**.

- 5 Click the **surface** tab to select that geometry.
- 6 From the **Options** menu, choose **Expressions>Subdomain Expressions**.
- 7 In the **Subdomain selection** list, select Subdomain 1.
- 8 Define the following subdomain expression (the term `c_bulk` is an extrusion-coupling variable that you define next); when done, click **OK**.

NAME	EXPRESSION
<code>react_surf</code>	<code>k_on*c_bulk*(R_t-B)-k_off*B</code>

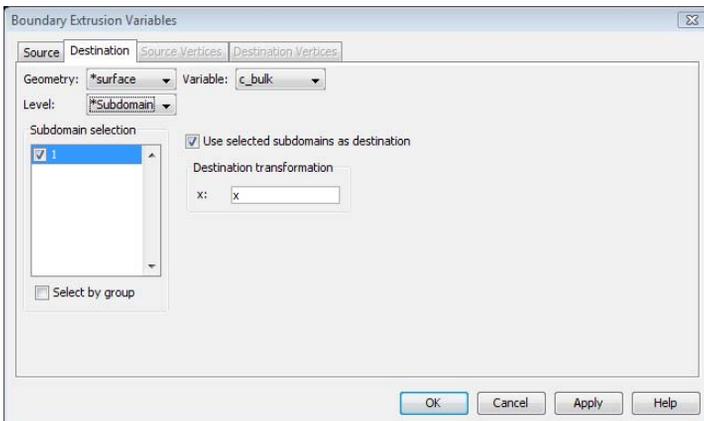
- 9 Click the **channel** tab to select that geometry.
- 10 From the **Options** menu, choose **Extrusion Coupling Variables>Boundary Variables**.
- 11 Select Boundary 5. In the first row of the **Name** column type `c_bulk`, then type `c` in the corresponding **Expression** column.
- 12 Click the **General transformation** option button.



Configuring the source of the extrusion coupling variable for the channel geometry.

- 13 Click the **Destination** tab.
- 14 From the **Geometry** list select **surface**, and from the **Level** list select **Subdomain**.

15 In the **Subdomain selection** list, click the check box to select Subdomain I. Make sure the **Use selected subdomains as destination** check box is selected.



Configuring the destination of the extrusion coupling variable for the channel geometry.

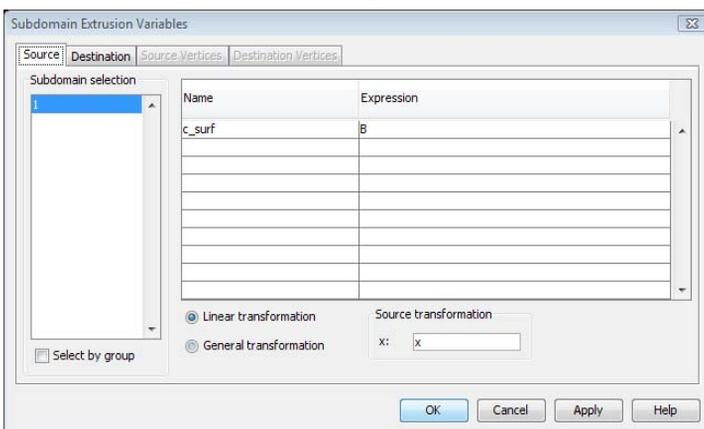
16 Click **OK**.

17 Verify that you still have the **surface** tab selected; if it is not selected, click it.

18 From the **Options** menu, choose **Extrusion Coupling Variables>Subdomain Variables**.

19 From the **Subdomain selection** list select **I**, go to the first row in the **Name** column and enter **c_surf**, then type **B** in the corresponding **Expression** column.

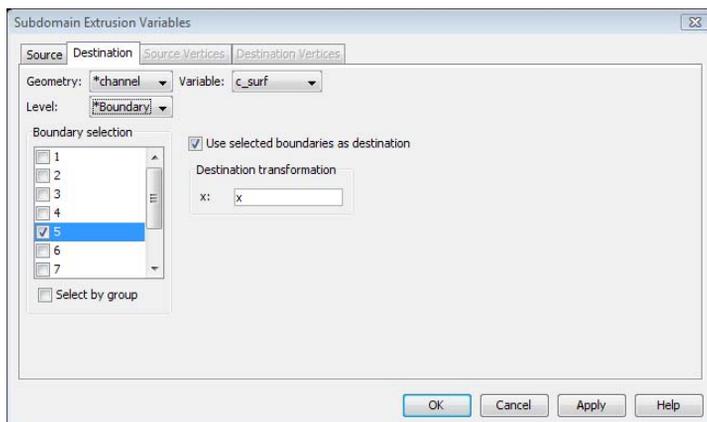
20 Click the **General transformation** option button.



Configuring the source of the extrusion coupling variable for the surface geometry.

21 Click the **Destination** tab.

- 22 From the **Geometry** list select **channel**, and from the **Level** list select **Boundary**.
- 23 In the **Boundary selection** list, click the check box to select Boundary 5. Make sure the **Use selected boundaries as destination** check box is selected.



Configuring the destination of the extrusion coupling variable for the surface geometry.

- 24 Click **OK**.

Finally set the integration-coupling variables needed for postprocessing. They represent the total amount of bonded molecules on the reaction surface and its length, respectively. Their ratio thus gives the average concentration of bonded molecules at the surface.

- 1 Select the **surface** geometry.
- 2 From the **Options** menu, select **Integration Coupling Variables>Subdomain Variables**.
- 3 Select Subdomain 1 and enter these settings:

NAME	EXPRESSION	INTEGRATION ORDER	GLOBAL DESTINATION
B_total	B	4	Selected
x_length	1	4	Selected

- 4 Click **OK**.

Subdomain Settings

- 1 From the **Multiphysics** menu, select **1 channel: Electrostatics (emes)**.
- 2 From the **Physics** menu, select **Subdomain Settings**.
- 3 Select Subdomain 1.

- 4 Under the options for the **Constitutive relation** click the option button corresponding to $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$.
- 5 In the **Relative permittivity** edit field type `epsilon_r_f`, then click **OK**.
- 6 From the **Multiphysics** menu, select **2 channel: Convection and Conduction (cc)**.
- 7 From the **Physics** menu, select **Subdomain Settings**.
- 8 Select Subdomain 1, then enter settings as in this table; when finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
k (isotropic)	<code>k_f</code>	Thermal conductivity
ρ	<code>rho_f</code>	Density
C_p	<code>Cp_f</code>	Heat capacity at constant pressure
Q	<code>sigma_f*normE_emes^2</code>	Heat source
u	<code>u</code>	x-velocity
v	<code>v</code>	y-velocity

- 9 From the **Multiphysics** menu, select **3 channel: Incompressible Navier-Stokes (mmglf)**.
- 10 From the **Physics** menu, select **Subdomain Settings**.
- 11 In the dialog box select Subdomain 1, then enter these settings:

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
ρ	<code>rho_f</code>	Density
η	<code>eta_f</code>	Dynamic viscosity
F_x	<code>Fx_et</code>	Volume force, x dir.
F_y	<code>Fy_et</code>	Volume force, x dir.

- 12 Click the **Init** tab. In the **x-velocity** edit field, type `u_av`. Click **OK**.
- 13 From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.
- 14 From the **Physics** menu, select **Subdomain Settings**.
- 15 Select Subdomain 1, then enter settings as in the following table; for the **Time-scaling coefficient** and the **Reaction rate**, leave the default settings. When finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
D (isotropic)	<code>D_a</code>	Diffusion coefficient
u	<code>u</code>	x-velocity
v	<code>v</code>	y-velocity

16 From the **Multiphysics** menu, choose **5 surface: Diffusion (di)**.

17 From the **Physics** menu, select **Subdomain Settings**.

18 Select Subdomain 1, then enter these settings; when finished, click **OK**.

QUANTITY	VALUE/EXPRESSION	DESCRIPTION
D	0	Diffusion coefficient
R	react_surf	Reaction rate

Boundary Conditions

1 From the **Multiphysics** menu, choose **1 channel: Electrostatics (emes)**.

2 From the **Physics** menu, select **Boundary Settings**.

3 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 4	BOUNDARY 8	BOUNDARIES 1-3, 5-7, 9, 10
Boundary condition	Electric potential	Electric potential	Zero charge/ Symmetry
V_0	$V_{rms}/2$	$-V_{rms}/2$	

4 From the **Multiphysics** menu, choose **2 channel: Convection and Conduction (cc)**.

5 From the **Physics** menu, select **Boundary Settings**.

6 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARIES 1, 10	BOUNDARIES 4, 8
Boundary condition	Heat flux	Temperature
q_0	$-k_f*(T-T_{amb})/l[mm] - n_x*u*rho_f*Cp_f*T$	
T_0		T_{amb}

The default boundary condition (thermal insulation) applies to the boundaries not listed in the table.

7 From the **Multiphysics** menu, select **3 channel: Incompressible Navier-Stokes (mmglf)**.

8 From the **Physics** menu, select **Boundary Settings**.

9 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 10	BOUNDARIES 2-9
Boundary type	Inlet	Outlet	Wall
Boundary condition	Laminar inflow	Pressure, no viscous stress	No slip

SETTINGS	BOUNDARY 1	BOUNDARY 10	BOUNDARIES 2-9
U_0	u_av		
L_{entr}	1 e - 4		
Constrain end points to zero	Yes		
P_0		0	

10 From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.

11 From the **Physics** menu, select **Boundary Settings**.

12 Enter boundary settings from the following table; when finished, click **OK**.

SETTINGS	BOUNDARY 1	BOUNDARY 5	BOUNDARY 10	BOUNDARIES 2-4, 6-9
Boundary condition	Concentration	Flux	Convective flux	Insulation/Symmetry
c_0	c_0			
N_0		react_bulk		

13 From the **Multiphysics** menu, select **5 surface: Diffusion (di)**.

14 From the **Physics** menu, select **Boundary Settings**.

15 Verify that the **Boundary condition** is set to **Insulation/Symmetry** on both boundaries.

16 Click **OK**.

MESH GENERATION

1 Select the **channel** geometry.

2 From the **Mesh** menu, select **Free Mesh Parameters**.

3 Click the **Boundary** tab.

4 Select Boundaries 4, 5, and 8.

5 In the **Maximum element size** edit field type $0.2e-6$.

6 Click the **Remesh** button to initialize the mesh for the **channel** geometry. Click **OK**.

7 Select the **surface** geometry.

8 Click the **Initialize Mesh** button on the Main toolbar to initialize the mesh for the **surface** geometry.

COMPUTING THE SOLUTION

You solve the model in three steps using three different solvers.

1 Click the **Solver Manager** button on the Main toolbar to launch the **Solver Manager**.

- 2 On the **Script** page, select the **Automatically add commands when solving** check box. With this setting, COMSOL Multiphysics records the subsequent solver commands so that you can reuse them when you later solve the model for $V_{\text{rms}} = 10 \text{ V}$.
- 3 On the **Solve For** page, select **channel (2D)>Electrostatics (emes)**.
- 4 Click **Solve**.
- 5 Click the **Initial Value** tab. In the **Values of variables not solved for and linearization point** area, select the **Current solution** option button.
- 6 Return to the **Solve For** page. Select the application modes **channel (2D)>Convection and Conduction (cc)** and **channel (2D)>Incompressible Navier-Stokes (mmglf)**.
- 7 Click **Solve**.
- 8 Click the **Solver Parameters** button on the Main toolbar to launch the **Solver Parameters** dialog box.
- 9 From the **Solver** list, select **Time dependent**.
- 10 On the **General** page, type 0:0.1:5 in the **Times** edit field in the **Time stepping** area.
- 11 Click **OK** to close the **Solver Parameters** dialog box.
- 12 Return to the **Solver Manager**.
- 13 On the **Solve For** page, select the application modes **channel (2D)>Convection and Diffusion (chcd)** and **surface (1D)>Diffusion (di)**.
- 14 Click **OK** to close the **Solver Manager** dialog box.
- 15 Click **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

Begin by visualizing the fluid flow and the analyte concentration in the flow channel after 5 s.

- 1 In the drawing area, select the **channel** geometry.
- 2 Click the **Plot Parameters** button on the Main toolbar.
- 3 On the **General** page of the **Plot Parameters** dialog box, select the check boxes for **Surface**, **Arrow**, **Streamline**, and **Geometry edges**. Make sure the **Solution at time** list is initialized to 5.
- 4 Click the **Surface** tab. From the **Predefined quantities** list, select **Convection and Diffusion (chcd)>Concentration, c**. In the **Unit** edit field, type umol/m^3 .
- 5 Click the **Arrow** tab. In the **Plot arrows on** list select **Subdomains**.
- 6 Click the **Subdomain Data** tab. From the **Predefined quantities** list, select **Incompressible Navier-Stokes (mmglf)>Velocity field**.

- 7 In the **Arrow parameters** area, find the **Arrow length** list and select **Proportional**.
- 8 Click the **Color** button. Select black, then click **OK** to close the **Arrow Color** dialog box.
- 9 Go to the **Streamline** page. Click the **Streamline Data** tab, then in the **Predefined quantities** list select **Incompressible Navier-Stokes (mmgIf)>Velocity field**.
- 10 From the **Streamline plot type** list, select **Magnitude controlled**.
- 11 Click the **Line Color** tab. Select the **Uniform color** option button. Click the **Color** button, then select the orange color corresponding to the RGB values (255, 102, 0). To do so, click the **RGB** tab and enter the values directly. Click **OK** to close the **Streamline Color** dialog box.
- 12 Return to the **General** page. From the **Plot in** list, select **New figure**.
- 13 Click **OK** to generate the plot in Figure 2 on page 8.

Next, generate the first graph in Figure 5 on page 9 with the following steps:

- 1 Select the **surface** geometry.
- 2 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
- 3 On the **General** page, verify that all solutions in the **Solutions to use** list are selected. From the **Plot in** list, select **New figure**.
- 4 Click the **Point** tab. In the **y-axis data** area, type B_{total}/x_{length} in the **Expression** edit field. In the **Coordinates** area, type $1e-4$ in the **x** edit field.
- 5 Click the **Line Settings** button. From the **Line marker** list select **Triangle**, then click **OK** to close the **Line Settings** dialog box.
- 6 Click **OK**.

Leave the figure windows open to enable comparison with the solutions for the case where an electric field has been applied.

Re-Solve the Model with an Applied Electric Field

In this second part of the modeling session, you apply an external electric field.

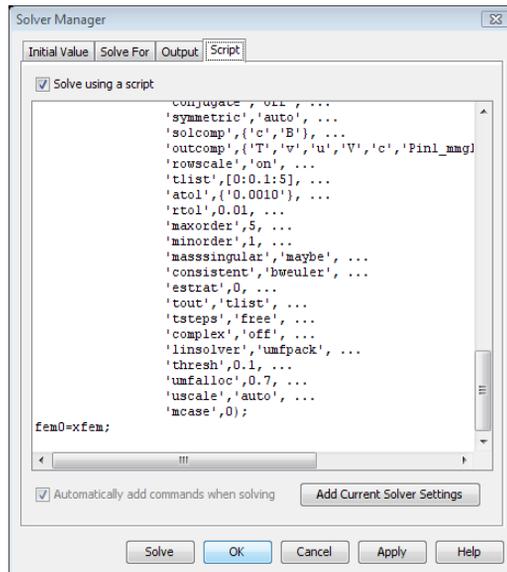
OPTIONS AND SETTINGS

Choose **Options>Constants**. Change the **Expression** for V_{rms} to $10[V]$, then click **OK**.

COMPUTING THE SOLUTION

- 1 Click the **Solver Manager** button on the Main toolbar.

- 2 On the **Script** page, select **Solve using a script** check box. The following solver script appears in the script area (the orders between the entries in the solcomp and outcomp lists can vary):



- 3 Click **OK** to close the **Solver Manager**.
- 4 Click the **Solve** button on the Main toolbar. The software automatically repeats all the solving stages you recorded in the first part of this model to compute the solution for $V_{\text{rms}} = 10$ V.

POSTPROCESSING AND VISUALIZATION

- 1 In the drawing area, select the **channel** geometry.
- 2 Click the **Plot Parameters** button on the Main toolbar.
- 3 On the **General** page, select **New figure** from the **Plot in** list. Click **Apply**.

The plot displayed in Figure 3 on page 8—visualizing the fluid flow and the analyte concentration in the flow channel after 5 s in the presence of an electric field—should now appear in the Figure 3 window. To plot the same quantities at $t = 1$ s, proceed with the following steps:

- 4 Still on the **General** page, from the **Solution at time** list select **1**.
- 5 From the **Plot in** list select **New figure**, then click **OK**.

The new figure window now contains a plot resembling that in Figure 4. This is the plot you see in the Model Navigator if you open the model from the Model Library.

Finally, finish reproducing Figure 5, which illustrates the binding rate of the analyte, by executing the following instructions:

- 1 Select the **surface** geometry.
- 2 From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
- 3 On the **Point** page, click the **Line Settings** button. From the **Line marker** list select **Square**, then click **OK** to close the **Line Settings** dialog box.
- 4 Click the **General** tab.
- 5 Select the **Keep current plot** check box.
- 6 Click the **Title/Axis** button.
- 7 Activate the **Title** edit field, then enter the title Average concentration of bonded molecules [mol/m^2].
The HTML tags produce a superscript figure “2” for the exponent.
- 8 Click **OK** to close the **Title/Axis Settings** dialog box.
- 9 Click **OK** to generate the plot.

The two graphs in the Figure 2 window should now look like those in Figure 5.

To study an animation of the solution, click the **Animate** button on the Plot toolbar.

Step-Response Simulation

OPTIONS AND SETTINGS

From the **Physics** menu, select **Constants**. Edit the expressions for the four last constants according to the following table; when done, click **OK**.

NAME	EXPRESSION
c0	75[$\mu\text{mol}/\text{m}^3$]
k_on	100[$\text{m}^3/(\text{mol}\cdot\text{s})$]
k_off	5e-3[1/s]
R_t	1.67e-11[mol/m^2]

PHYSICS SETTINGS

- 1 From the **Multiphysics** menu, select **4 channel: Convection and Diffusion (chcd)**.
- 2 From the **Physics** menu, select **Boundary Settings**. Select Boundary 1.

- 3 Change the entry in the c_0 edit field to $c_0*(t < 1000[s])$, then click **OK**.

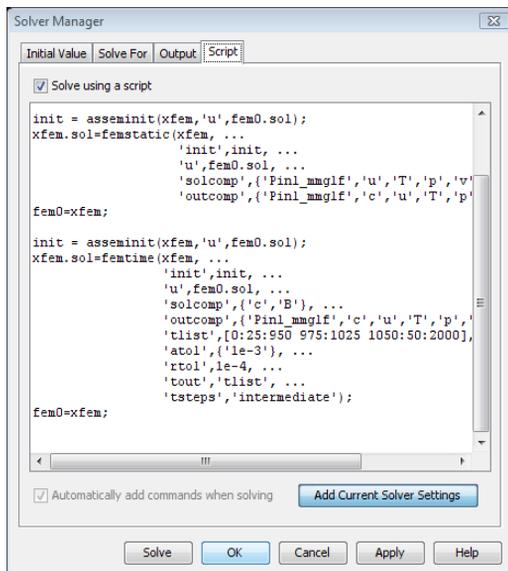
The logical expression implements the step function in Equation 3.

COMPUTING THE SOLUTION

- 1 Click the **Solver Parameters** button on the Main toolbar.
- 2 Change the entry in the **Times** edit field to 0:25:950 975:1025 1050:50:2000.
- 3 Set the **Relative tolerance** to $1e-4$ and the **Absolute tolerance** to $1e-3$.
- 4 Click the **Time Stepping** tab.
- 5 From the **Time steps taken by solver** list, select **Intermediate**.
- 6 Click **OK** to close the **Solver Parameters** dialog box.
- 7 Click the **Solver Manager** button on the Main toolbar.
- 8 On the **Script** page, click the **Add Current Solver Settings** button.

A `femtime` command with the current solver settings appears in the script area.

- 9 Because this command should replace the previous one, cut out the complete *upper* `femtime` command together with the `assemnit` command line immediately before it as well as the `fem0=xfem;` line immediately after it. When you are done, the contents of the script area should be as in the following figure (again, the entries in the `solcomp` and `outcomp` lists can be ordered differently).



10 Click **OK** to close the **Solver Manager**.

11 Click the **Solve** button on the Main toolbar.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 6, follow these steps:

- 1** Select the **surface** geometry.
- 2** From the **Postprocessing** menu, select **Cross-Section Plot Parameters**.
- 3** On the **General** page, select **New figure** from the **Plot in** list.
- 4** On the **Point** page, click the **Line Settings** button. From the **Line marker** list select **None**, then click **OK** to close the **Line Settings** dialog box.
- 5** Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the plot.