



Model created in COMSOL Multiphysics 6.4

# Simulation of an Ion-Sensitive Field-Effect Transistor (ISFET)



This tutorial uses a 2D model of an ion-sensitive field-effect transistor (ISFET) to illustrate the basic steps to set up the coupling between semiconductor physics and electrochemistry.

### *Introduction*

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An ion-sensitive field-effect transistor (ISFET) is constructed by replacing the gate contact of a MOSFET with an electrolyte of interest. The concentration of a specific ionic species in the electrolyte can be determined by measuring the change in the gate voltage due to the interaction between the ions and the gate dielectric. This tutorial of an ISFET pH sensor illustrates the procedure to set up the coupling between the semiconductor model and the electrolyte model. It also shows the technique of using a simple global equation to extract operating parameters without the need of explicit modeling of the actual feedback circuitry.

### *Model Definition*

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The model is composed of essentially two adjacent domains: a semiconductor domain and an electrolyte domain. (The electrolyte domain is split in half along the centerline of the geometry for convenience in making some graphs.) The semiconductor domain is set up as a MOSFET. The thin oxide layer is not explicitly modeled — the dedicated **Thin Insulator Gate** boundary condition is used instead. Unlike a conventional MOSFET, the electric potential at the outer surface of the oxide ( $\phi_M$ ) is not given by the potential of a metal contact; rather, it is given by the electric potential of the electrolyte just outside of the Stern layer, plus the voltage drop across the Stern layer, following the same treatment as in the Diffuse Double Layer tutorial.

The electrolyte domain is set up in the same way as the Diffuse Double Layer tutorial except that the Transport of Charge Carriers interface is used instead, with the addition of hydronium and hydroxide ions. The Stern layer is not explicitly modeled — a simple formula relating the electric potential on each side of the Stern layer is used instead. The bulk electrolyte potential is given by a simple formula combining the gate voltage applied on the reference electrode (not explicitly modeled), the work function of the electrode metal, and the equilibrium potential of the reference electrode. Unlike in the tutorial, the value of the electric potential at the outer surface of the oxide ( $\phi_M$ ) is not given by a prescribed constant; rather, it is solved for in a self-consistent manner. The self-consistent set of equations include essentially three parts:

- $\phi_M$  is the sum of the voltage drop across the Stern layer and the electrolyte potential just outside of the Stern layer.

- The charge density on the oxide surface is given by the equilibrium reaction between protons and the proton binding sites on the oxide surface.
- The chemical activity of the protons on the oxide surface is related to the hydronium ion concentration in the bulk electrolyte via the Boltzmann distribution function. This treatment follows the approach given in Ref. 1. A user can of course choose to implement a different theory for this much-debated area of surface electrochemistry.

The coupling between the semiconductor and the electrolyte domain is implemented as the following. For the semiconductor domain, the electric potential  $\phi_M$  is imposed on the oxide surface. For the electrolyte domain, the displacement field is determined from the charge density on the oxide surface and the displacement field on the semiconductor side using Gauss' law, and imposed on the boundary. Note that it is assumed that there is no space charge in the Stern layer; therefore, the displacement field does not change across the Stern layer.

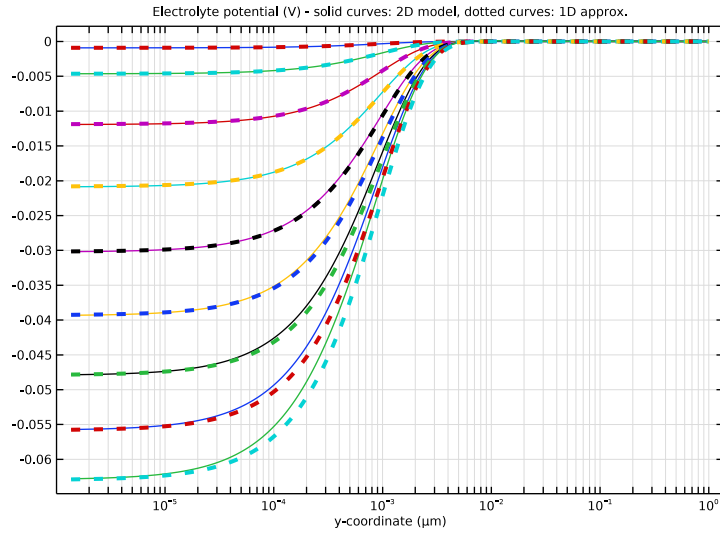
As the fully coupled system is highly nonlinear, individual studies are set up in a sequence to solve different aspects of the system step by step, using the solution from each previous study as the initial condition for the next study. First only the electrolyte part is solved. Then the semiconductor part is solved. Then the fully coupled system is solved in three different scenarios, to examine:

- 1 The drain current as a function of the applied gate voltage.
- 2 The drain current — drain voltage curve for three different pH values.
- 3 The gate voltage as a function of the pH value in the real operating condition where a feedback circuit adjusts the gate voltage to keep the drain current constant. In the last study, a global equation is used to mimic the effect of the feedback circuit, which is not explicitly modeled.

## *Results and Discussion*

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Figure 1 shows the electrolyte potential along the centerline of the electrolyte domain, comparing the simulation result (solid curves) and the 1D approximation formula (dotted curves; Ref. 1). The 1D approximation formula matches the general trend of the 2D model result.



*Figure 1: Electrolyte potential along the centerline of the electrolyte domain. (It does not extrapolate to the dielectric surface potential at  $y=0$  because the voltage drop across the Stern layer is not explicitly modeled in the electrolyte domain. See [Model Definition](#) for details.)*

Figure 2 shows the drain current as a function of the gate voltage for the fully coupled system. The behavior of this  $I_d$ - $V_g$  curve is essentially the same as a regular MOSFET. This is expected since the electrolyte acts as a conductor to transmit the applied voltage to the oxide surface, albeit with a more complicated mechanism than a simple metal contact.

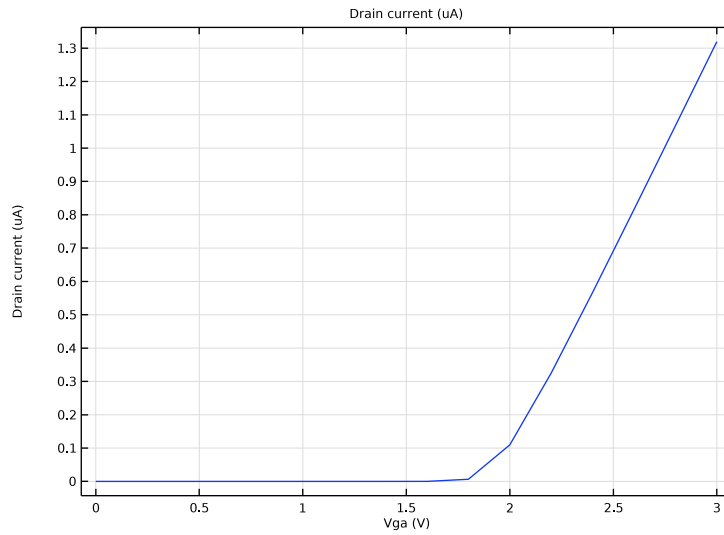


Figure 2: Drain current as a function of the applied gate voltage.

Figure 3 shows the drain current–drain voltage curves for three different pH values. Again the behavior of the family of curves looks just like a regular MOSFET, except for the fact that in a regular MOSFET the control parameter is the gate voltage but here the control parameter is the pH value.

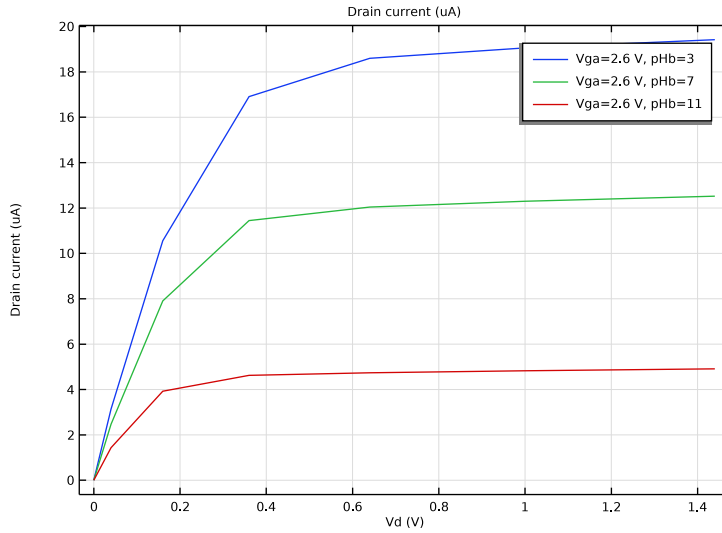


Figure 3: Drain current–drain voltage curves for three different pH values.

Figure 4 shows the sensitivity curve for the ISFET pH sensor operating in the constant-current mode, where a feedback circuit adjusts the applied gate voltage such that the drain current is maintained at a constant set point. The resulting gate voltage (the output of the sensor) as a function of the pH value (the input of the sensor) is plotted in the figure. The slope of the curve gives the sensitivity, which is consistent with the one reported in Ref. 1.

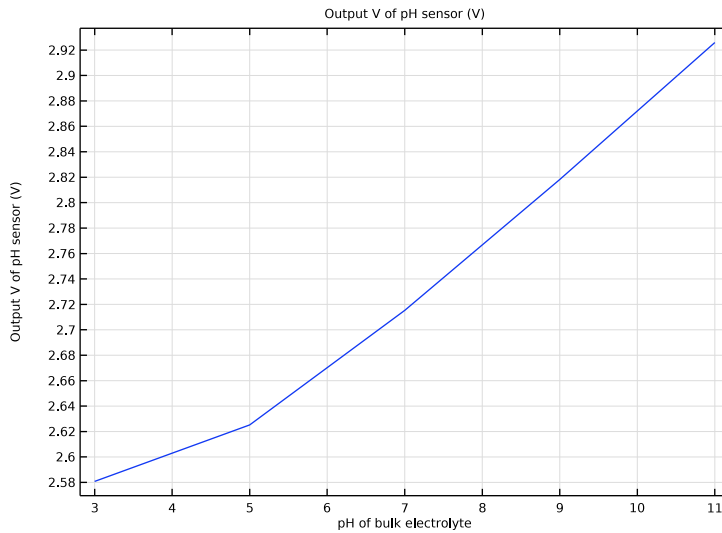


Figure 4: Sensitivity curve for the ISFET pH sensor.

### Reference

1. R.E.G. van Hal, J.C.T. Eijkel, P. Bergveld, A general model to describe the electrostatic potential at electrolyte oxide interfaces, *Advances in Colloid and Interface Science*, Volume 69, Issue 1, 1996, Pages 31-62, ISSN 0001-8686, [http://dx.doi.org/10.1016/S0001-8686\(96\)00307-7](http://dx.doi.org/10.1016/S0001-8686(96)00307-7). (<http://www.sciencedirect.com/science/article/pii/S0001868696003077>)

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**Application Library path:** Semiconductor\_Module/  
 Photonic\_Devices\_and\_Sensors/isfet

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### 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 **Semiconductor > Semiconductor (semi)**.
- 3 Click **Add**.
- 4 Click  **Done**.

Studies will be added later.

## GEOMETRY I


The Model Wizard starts the COMSOL Desktop with the **Geometry** node selected. Take the opportunity to set the length unit to a more convenient one.

- 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 **μm**.

Now import some global parameters from a text file.

## GLOBAL DEFINITIONS


### *Parameters 1*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `isfet_parameters.txt`.


Next build the geometric objects in the model.

## GEOMETRY I

### *Rectangle 1 (r1)*

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type 3.
- 4 In the **Height** text field, type 0.7.
- 5 Locate the **Position** section. In the **y** text field, type -0.7.


### *Polygon 1 (pol1)*

- 1 In the **Geometry** toolbar, click  **Polygon**.

- 2 In the **Settings** window for **Polygon**, locate the **Object Type** section.
- 3 From the **Type** list, choose **Closed curve**.
- 4 Locate the **Coordinates** section. In the table, enter the following settings:


x ( $\mu\text{m}$ )	y ( $\mu\text{m}$ )
0	-0.03
0	0
0.5	0
2.5	0
3	0
3	-0.03

*Polygon 2 (pol2)*

- 1 In the **Geometry** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
- 3 In the table, enter the following settings:

x ( $\mu\text{m}$ )	y ( $\mu\text{m}$ )
0	1
0.7	0
2.3	0
3	1

*Polygon 3 (pol3)*

- 1 In the **Geometry** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Object Type** section.
- 3 From the **Type** list, choose **Open curve**.
- 4 Locate the **Coordinates** section. In the table, enter the following settings:

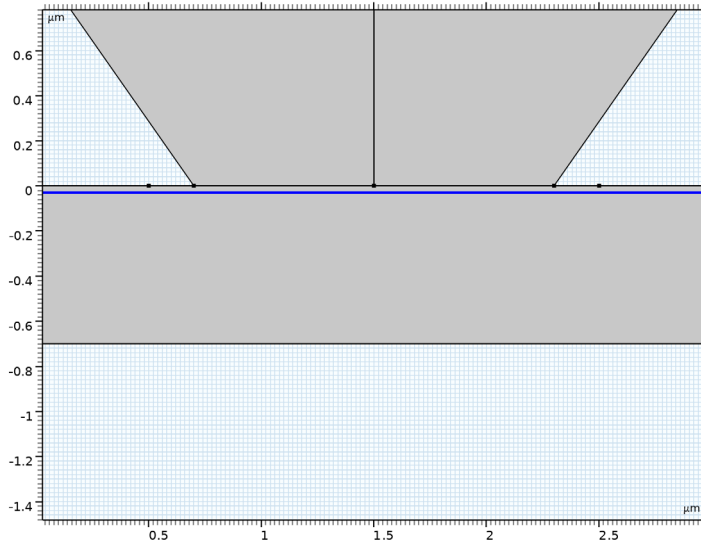
x ( $\mu\text{m}$ )	y ( $\mu\text{m}$ )
1.5	0
1.5	1

*Mesh Control Edges 1 (mce1)*

- 1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundary 4 only.

It might be easier to select the correct boundary by using the **Selection List** window. To open this window, in the **Home** toolbar click **Windows** and choose **Selection List**. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)



Define some variables to be used in various stages of the model setup.

### DEFINITIONS

*Variables for applying specified gate voltage ( $V_g$ )*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables for applying specified gate voltage ( $V_g$ ) in the **Label** text field.
- 3 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
phil_bulk_g	Vga-WAg-Eeq	V	Bulk electrolyte potential

*Variables for adjusting  $V_g$  to obtain specified drain current*

- 1 Right-click **Variables for applying specified gate voltage ( $V_g$ )** and choose **Duplicate**.
- 2 In the **Settings** window for **Variables**, type Variables for adjusting  $V_g$  to obtain specified drain current in the **Label** text field.

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

Name	Expression	Unit	Description
phil_bulk_d	Vg-WAg-Eeq		Bulk electrolyte potential

*Variables on oxide surface*



- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables on oxide surface in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 Select Boundaries 7 and 9 only.
- 5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
aHs_g	$cH\_bulk \cdot \exp(-(\phi_M - \phi_{il\_bulk\_g})/V\_therm)$		Activity of H <sup>+</sup>
rhos0_g	$e\_const \cdot N_s \cdot (aHs\_g^2 - K_a \cdot K_b) / (K_a \cdot K_b + K_b \cdot aHs\_g + aHs\_g^2)$		Surface charge density
aHs_d	$cH\_bulk \cdot \exp(-(\phi_M - \phi_{il\_bulk\_d})/V\_therm)$		Activity of H <sup>+</sup>
rhos0_d	$e\_const \cdot N_s \cdot (aHs\_d^2 - K_a \cdot K_b) / (K_a \cdot K_b + K_b \cdot aHs\_d + aHs\_d^2)$		Surface charge density

Some expressions entered so far may contain undefined variables and turn to yellow color. The missing variables will be defined later and the color for the expressions will turn back to black.


Define materials.

#### ADD MATERIAL

- 1 In the **Home** toolbar, click  **Add Material** to open the **Add Material** window.
- 2 Go to the **Add Material** window.
- 3 In the tree, select **Semiconductors > Si - Silicon**.
- 4 Click the **Add to Component** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## MATERIALS

### *Electrolyte*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, type **Electrolyte** in the **Label** text field.
- 3 Select Domains 2 and 3 only.
- 4 Locate the **Geometric Entity Selection** section. Click  **Create Selection**.
- 5 In the **Create Selection** dialog, type **Electrolyte** domains in the **Selection name** text field.
- 6 Click **OK**.
- 7 In the **Settings** window for **Material**, locate the **Material Contents** section.
- 8 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilon <sub>r_</sub> iso ; epsilon <sub>r</sub> ii = epsilon <sub>r_</sub> iso, epsilon <sub>r</sub> ij = 0	eps_H2O	1	Basic

So far all domains are assigned to the **Semiconductor** interface. Therefore, there are red marks for the electrolyte material properties. Once the proper physics is assigned to the electrolyte domain, the unnecessary material property entries and the red marks should disappear.

Set up the semiconductor domain and boundary conditions, similar to the MOSFET tutorial in the Application Libraries.

## SEMICONDUCTOR (SEMI)


- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Semiconductor (semi)**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Semiconductor**, locate the **Model Properties** section.
- 4 From the **Carrier statistics** list, choose **Fermi–Dirac**.

### *Semiconductor Material Model 1*


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Semiconductor (semi)** click **Semiconductor Material Model 1**.
- 2 In the **Settings** window for **Semiconductor Material Model**, locate the **Model Input** section.

3 In the  $T$  text field, type T0.

*Uniform background doping*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Analytic Doping Model**.
- 2 In the **Settings** window for **Analytic Doping Model**, type Uniform background doping in the **Label** text field.
- 3 Select Domain 1 only.
- 4 Locate the **Impurity** section. In the  $N_{A0}$  text field, type  $1e17[1/cm^3]$ .

*Source doping*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Analytic Doping Model**.
- 2 In the **Settings** window for **Analytic Doping Model**, type Source doping in the **Label** text field.
- 3 Select Domain 1 only.
- 4 Locate the **Distribution** section. From the list, choose **Box**.
- 5 Locate the **Impurity** section. From the **Impurity type** list, choose **Donor doping (n-type)**.
- 6 In the  $N_{D0}$  text field, type  $1e20[1/cm^3]$ .
- 7 Locate the **Uniform Region** section. Specify the  $r_0$  vector as

-0.1[um]	Y
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- 8 In the  $W$  text field, type  $0.6[um]$ .
- 9 In the  $D$  text field, type  $0.1[um]$ .
- 10 Locate the **Profile** section. Select the **Specify different length scales for each direction** checkbox.
- 11 Specify the  $d_j$  vector as

0.2[um]	X
0.25[um]	Y

The background doping level for the junction profile can be conveniently set to the uniform background doping level that you just defined, using the **Background doping concentration** list.


- 12 From the  $N_b$  list, choose **Acceptor concentration (semi/adm1)**.
- 13 To see which item in the list corresponds to which node in the model tree, toggle on the **Tag** setting in the **Model Tree Node Text** menu in the **Model Builder** window toolbar.

#### Drain doping


- 1 Right-click **Source doping** and choose **Duplicate**.
- 2 In the **Settings** window for **Analytic Doping Model**, type Drain doping in the **Label** text field.
- 3 Locate the **Uniform Region** section. Specify the  $r_0$  vector as

2.4[um]	X
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#### Trap-Assisted Recombination 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **Trap-Assisted Recombination**.
- 2 Select Domain 1 only.


#### Source

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Metal Contact**.
- 2 In the **Settings** window for **Metal Contact**, type Source in the **Label** text field.
- 3 Select Boundary 3 only.


#### Drain

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Metal Contact**.
- 2 In the **Settings** window for **Metal Contact**, type Drain in the **Label** text field.
- 3 Select Boundary 13 only.
- 4 Locate the **Terminal** section. In the  $V_0$  text field, type  $V_d$ .

#### Body


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Metal Contact**.
- 2 In the **Settings** window for **Metal Contact**, type Body in the **Label** text field.
- 3 Select Boundary 2 only.

#### Thin Insulator Gate 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Thin Insulator Gate**.
- 2 Select Boundaries 7 and 9 only.
- 3 In the **Settings** window for **Thin Insulator Gate**, locate the **Terminal** section.
- 4 In the  $V_0$  text field, type  $\phi_{iM}$ .
- 5 Locate the **Gate Contact** section. In the  $\epsilon_{ins}$  text field, type 4.5.
- 6 In the  $d_{ins}$  text field, type 30[nm].
- 7 In the  $\Phi$  text field, type 0[V].

The undefined variable  $\phi_{iM}$  will be defined later.

### ADD PHYSICS

- 1 In the **Physics** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **AC/DC** > **Electric Fields and Currents** > **Electrostatics (es)**.
- 4 Click to expand the **Dependent Variables** section. In the **Electric potential (V)** text field, type `phi1`.
- 5 Click the **Add to Component 1** button in the window toolbar.


### ELECTROSTATICS (ES)

- 1 In the **Settings** window for **Electrostatics**, locate the **Domain Selection** section.
- 2 From the **Selection** list, choose **Electrolyte domains**.

### ADD PHYSICS

- 1 Go to the **Add Physics** window.
- 2 In the tree, select **Electric Discharge** > **Transport of Charge Carriers (tcc)**.
- 3 Click the **Add to Component 1** button in the window toolbar.

### TRANSPORT OF CHARGE CARRIERS (ELECTROLYTE)

- 1 In the **Settings** window for **Transport of Charge Carriers**, type `Transport of Charge Carriers (electrolyte)` in the **Label** text field.
- 2 Locate the **Domain Selection** section. In the list box, select **1**.
- 3 Click  **Remove from Selection**.
- 4 Select Domains 2 and 3 only.
- 5 From the **Selection** list, choose **Electrolyte domains**.
- 6 Locate the **Physical Model** section. In the  $d_z$  text field, type `1 [m]`.
- 7 Click to expand the **Dependent Variables** section. In the **Number of charge carriers** text field, type `4`.
- 8 In the **Charge carriers (1/m<sup>3</sup>)** table, enter the following settings:

<hr/>
C
<hr/>
A
<hr/>
H
<hr/>
OH
<hr/>

### ADD PHYSICS


- 1 Go to the **Add Physics** window.
- 2 In the tree, select **Mathematics > ODE and DAE Interfaces > Boundary ODEs and DAEs (bode)**.
- 3 Click to expand the **Dependent Variables** section. In the **Dependent variables (1)** table, enter the following settings:

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$\phi_{iM}$

- 4 Click the **Add to Component 1** button in the window toolbar.

### BOUNDARY ODES AND DAES (BODE)

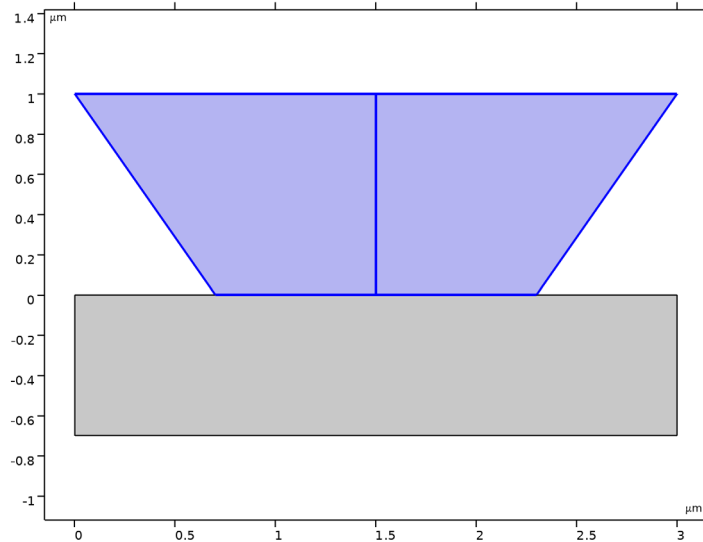
- 1 In the **Settings** window for **Boundary ODEs and DAEs**, locate the **Boundary Selection** section.
- 2 Click  **Clear Selection**.
- 3 Select Boundaries 7 and 9 only.

### ADD PHYSICS

- 1 Go to the **Add Physics** window.
- 2 In the tree, select **Mathematics > ODE and DAE Interfaces > Global ODEs and DAEs (ge)**.
- 3 Click the **Add to Component 1** button in the window toolbar.
- 4 In the tree, select **Mathematics > ODE and DAE Interfaces > Global ODEs and DAEs (ge)**.
- 5 Click the **Add to Component 1** button in the window toolbar.
- 6 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.


## ELECTROSTATICS (ELECTROLYTE)

- 1 In the **Settings** window for **Electrostatics**, type Electrostatics (electrolyte) in the **Label** text field.





- 2 Locate the **Thickness** section. In the  $d$  text field, type  $1e-6$ [m].

### Charge Conservation in Fluids I

- 1 In the **Physics** toolbar, click  **Domains** and choose **Charge Conservation in Fluids**.
- 2 In the **Settings** window for **Charge Conservation in Fluids**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Electrolyte domains**.

## BOUNDARY ODE FOR OXIDE SURFACE POTENTIAL PHIM

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Boundary ODEs and DAEs (bode)**.
- 2 In the **Settings** window for **Boundary ODEs and DAEs**, type Boundary ODE for oxide surface potential  $\phi_{iM}$  in the **Label** text field.
- 3 Locate the **Units** section. Click  **Select Dependent Variable Quantity**.
- 4 In the **Physical Quantity** dialog, type electricpotential in the text field.
- 5 In the tree, select **Electromagnetics > Electric potential (V)**.
- 6 Click **OK**.
- 7 In the **Settings** window for **Boundary ODEs and DAEs**, locate the **Units** section.

- 8 Click  **Select Source Term Quantity**.
- 9 In the **Physical Quantity** dialog, type electricpotential in the text field.
- 10 In the tree, select **Electromagnetics > Electric potential (V)**.
- 11 Click **OK**.

#### **GLOBAL ODE TO COPY SPECIFIED VG VALUE**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Global ODEs and DAEs (ge)**.
- 2 In the **Settings** window for **Global ODEs and DAEs**, type Global ODE to copy specified Vg value in the **Label** text field.

#### **GLOBAL ODE TO ADJUST VG FOR SPECIFIED DRAIN CURRENT**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Global ODEs and DAEs 2 (ge2)**.
- 2 In the **Settings** window for **Global ODEs and DAEs**, type Global ODE to adjust Vg for specified drain current in the **Label** text field.


Toggle off the **Add Physics** window.

Set up the electrostatics physics for the electrolyte.


#### **ELECTROSTATICS (ELECTROLYTE) (ES)**

In the **Model Builder** window, under **Component 1 (comp1)** click **Electrostatics (electrolyte) (es)**.

##### *Electric Potential 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Potential**.
- 2 Select Boundaries 5 and 10 only.
- 3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.
- 4 In the  $V_0$  text field, type phil\_bulk\_g.

##### *Electric Potential 2*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Potential**.
- 2 Select Boundaries 5 and 10 only.
- 3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.
- 4 In the  $V_0$  text field, type phil\_bulk\_d.


##### *Electric Displacement Field from semiconductor side*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Displacement Field**.


- 2 In the **Settings** window for **Electric Displacement Field**, type Electric Displacement Field from semiconductor side in the **Label** text field.
- 3 Select Boundaries 7 and 9 only.
- 4 Locate the **Electric Displacement Field** section. Specify the  $\mathbf{D}_0$  vector as

$\text{semi.nD\_ins*semi.nX}$	x
$\text{semi.nD\_ins*semi.nY}$	y


#### *Surface Charge Density 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Surface Charge Density**.
- 2 Select Boundaries 7 and 9 only.
- 3 In the **Settings** window for **Surface Charge Density**, locate the **Surface Charge Density** section.
- 4 In the  $\rho_s$  text field, type rhos0\_g.

#### *Surface Charge Density 2*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Surface Charge Density**.
- 2 Select Boundaries 7 and 9 only.
- 3 In the **Settings** window for **Surface Charge Density**, locate the **Surface Charge Density** section.
- 4 In the  $\rho_s$  text field, type rhos0\_d.

#### *Space Charge Density 1*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Space Charge Density**.
- 2 In the **Settings** window for **Space Charge Density**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Space Charge Density** section. From the  $\rho_v$  list, choose **Space charge density (tcc/tp1)**.

Set up the transport physics for the electrolyte.

### **TRANSPORT OF CHARGE CARRIERS (ELECTROLYTE) (TCC)**

#### *Transport Properties 1*


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport of Charge Carriers (electrolyte) (tcc)** click **Transport Properties 1**.
- 2 In the **Settings** window for **Transport Properties**, locate the **Electric Field** section.
- 3 From the **E** list, choose **Electric field (es)**.

- 4 Locate the **Drift** section. In the  $z_C$  text field, type  $z_C$ .
- 5 In the  $z_A$  text field, type  $z_A$ .
- 6 In the  $z_H$  text field, type 1.
- 7 In the  $z_{OH}$  text field, type -1.
- 8 In the  $\mu_C$  text field, type  $DC * F\_const / (R\_const * T0)$ .
- 9 In the  $\mu_A$  text field, type  $DA * F\_const / (R\_const * T0)$ .
- 10 In the  $\mu_H$  text field, type  $DH * F\_const / (R\_const * T0)$ .
- 11 In the  $\mu_{OH}$  text field, type  $DOH * F\_const / (R\_const * T0)$ .
- 12 Locate the **Diffusion** section. In the  $D_C$  text field, type  $DC$ .
- 13 In the  $D_A$  text field, type  $DA$ .
- 14 In the  $D_H$  text field, type  $DH$ .
- 15 In the  $D_{OH}$  text field, type  $DOH$ .



#### *Initial Values I*

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the  $n_C$  text field, type  $cC\_bulk * N\_A\_const$ .
- 4 In the  $n_A$  text field, type  $cA\_bulk * N\_A\_const$ .
- 5 In the  $n_H$  text field, type  $cH\_bulk * N\_A\_const$ .
- 6 In the  $n_{OH}$  text field, type  $cOH\_bulk * N\_A\_const$ .

#### *No Flux I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **No Flux**.
- 2 In the **Settings** window for **No Flux**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **All boundaries**.

#### *Number Density I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Number Density**.
- 2 In the **Settings** window for **Number Density**, locate the **Boundary Selection** section.
- 3 Click  **Paste Selection**.
- 4 In the **Paste Selection** dialog, type 5 10 in the **Selection** text field.
- 5 Click **OK**.
- 6 In the **Settings** window for **Number Density**, locate the **Number Density** section.
- 7 Select the **Carrier C** checkbox.

- 8** In the  $n_{0,C}$  text field, type  $cC\_bulk*N\_A\_const$ .
- 9** Select the **Carrier A** checkbox.
- 10** In the  $n_{0,A}$  text field, type  $cA\_bulk*N\_A\_const$ .
- 11** Select the **Carrier H** checkbox.
- 12** In the  $n_{0,H}$  text field, type  $cH\_bulk*N\_A\_const$ .
- 13** Select the **Carrier OH** checkbox.
- 14** In the  $n_{0,OH}$  text field, type  $cOH\_bulk*N\_A\_const$ .

Set up the boundary equation at the oxide surface. This couples the electric potential at the surface of the oxide to the electrolyte potential just outside of the Stern layer.

#### **BOUNDARY ODE FOR OXIDE SURFACE POTENTIAL $\phi_{iM}$ (BODE)**

##### *Distributed ODE 1*

- 1** In the **Model Builder** window, under **Component 1 (comp1) > Boundary ODE for oxide surface potential  $\phi_{iM}$  (bode)** click **Distributed ODE 1**.
- 2** In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.
- 3** In the  $f$  text field, type  $\phi_{i1}+es.nD/Ci\_st-\phi_{iM}$ .
- 4** Locate the **Damping or Mass Coefficient** section. In the  $d_a$  text field, type 0.

##### *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  $\phi_{iM}$  text field, type  $\phi_{i1\_bulk\_g}-0.01[V]$ .

##### *Initial Values 2*

- 1** Right-click **Component 1 (comp1) > Boundary ODE for oxide surface potential  $\phi_{iM}$  (bode) > Initial Values 1** and choose **Duplicate**.
- 2** In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3** In the  $\phi_{iM}$  text field, type  $\phi_{i1\_bulk\_d}-0.01[V]$ .


Set up the two global equations for the gate voltage. Depending on the goal of each study, at most one of the two will be used at the same time.

## GLOBAL ODE TO COPY SPECIFIED VG VALUE (GE)

### Global Equations 1 (ODE1)


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Global ODE to copy specified Vg value (ge)** click **Global Equations 1 (ODE1)**.
- 2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.
- 3 In the table, enter the following settings:

Name	f(u,ut,utt, t) (I)	Initial value (u_0) (I)	Initial value (ut_0) (I/s)	Description
Vg	(Vg - Vga) / 1 [V]	0	0	

- 4 Locate the **Units** section. Click  **Select Dependent Variable Quantity**.
- 5 In the **Physical Quantity** dialog, type electricpotential in the text field.
- 6 In the tree, select **Electromagnetics** > **Electric potential (V)**.
- 7 Click **OK**.

## GLOBAL ODE TO ADJUST VG FOR SPECIFIED DRAIN CURRENT (GE2)

### Global Equations 1 (ODE2)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Global ODE to adjust Vg for specified drain current (ge2)** click **Global Equations 1 (ODE2)**.
- 2 In the **Settings** window for **Global Equations**, locate the **Units** section.
- 3 Click  **Select Dependent Variable Quantity**.
- 4 In the **Physical Quantity** dialog, type electricpotential in the text field.
- 5 In the tree, select **Electromagnetics** > **Electric potential (V)**.
- 6 Click **OK**.
- 7 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.
- 8 In the table, enter the following settings:

Name	f(u,ut,utt, t) (I)	Initial value (u_0) (V)	Initial value (ut_0) (V/s)	Description
Vg	semi.IO_2 / 18 [uA] - 1	0	0	

Construct the mesh. Use **Mapped** mesh and **Boundary Layers** to minimize the number of mesh elements while keeping the required resolution near the oxide surface.

#### **MESH 1**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.
- 3 From the list, choose **User-controlled mesh**.

#### *Size*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Mesh 1** click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type  $h_{max}$ .

#### *Size 1*

- 1 In the **Model Builder** window, click **Size 1**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section.
- 5 Select the **Maximum element growth rate** checkbox. In the associated text field, type 1.05.

#### *Size 2*

In the **Model Builder** window, right-click **Size 2** and choose **Delete**.


#### *Size 3*

Right-click **Size 3** and choose **Delete**.

#### *Free Triangular 1*

Right-click **Free Triangular 1** and choose **Delete**.


#### *Edge 1*

- 1 In the **Mesh** toolbar, click  **More Generators** and choose **Edge**.
- 2 Select Boundaries 3, 6, 7, 9, 11, and 13 only.
- 3 In the **Settings** window for **Edge**, click to expand the **Control Entities** section.
- 4 From the **Smooth across removed control entities** list, choose **Off**.

### *Size 1*

- 1 Right-click **Edge 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **Semiconductor**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section.
- 6 Select the **Maximum element size** checkbox. In the associated text field, type 0.03.

### *Mapped 1*

- 1 In the **Mesh** toolbar, click  **Mapped**.
- 2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 4 only.
- 5 Click to expand the **Control Entities** section. From the **Smooth across removed control entities** list, choose **Off**.
- 6 Click to expand the **Reduce Element Skewness** section. Select the **Adjust edge mesh** checkbox.


### *Distribution 1*

- 1 Right-click **Mapped 1** and choose **Distribution**.
- 2 Select Boundary 15 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type 8.
- 6 In the **Element ratio** text field, type 9.
- 7 From the **Growth rate** list, choose **Exponential**.
- 8 Select the **Reverse direction** checkbox.

### *Free Triangular 1*

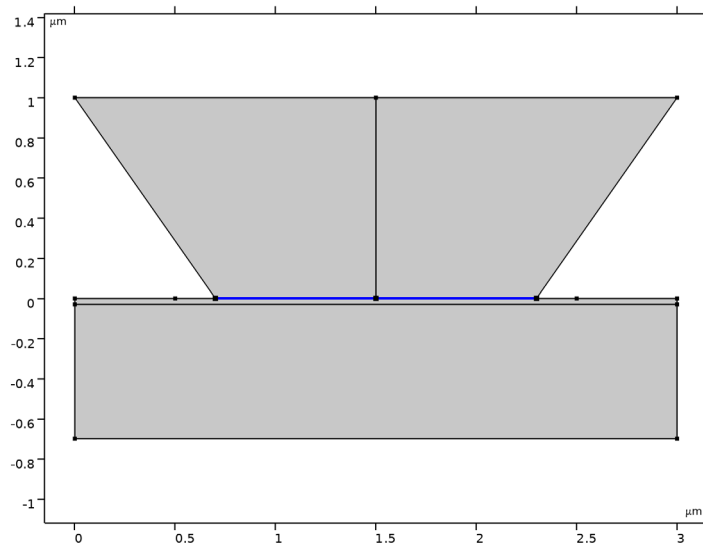
- 1 In the **Mesh** toolbar, click  **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 1 only.
- 5 Click to expand the **Control Entities** section. From the **Smooth across removed control entities** list, choose **Off**.

### Boundary Layers I

- 1 In the **Mesh** toolbar, click  **Boundary Layers**.
- 2 In the **Settings** window for **Boundary Layers**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Electrolyte domains**.

### Boundary Layer Properties


- 1 In the **Model Builder** window, click **Boundary Layer Properties**.
- 2 Select Boundaries 7 and 9 only.



- 3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.
- 4 In the **Number of layers** text field, type 20.
- 5 In the **Stretching factor** text field, type 1.3.
- 6 From the **Thickness specification** list, choose **First layer**.
- 7 In the **Thickness** text field, type  $h_{\max\_surf}$ .

Now set up the studies. First let us only look at the electrolyte.








### ADD STUDY

- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.

- 3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Semiconductor (semi)**, **Global ODE to copy specified Vg value (ge)**, and **Global ODE to adjust Vg for specified drain current (ge2)**.
- 4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Stationary**.
- 5 Click the **Add Study** button in the window toolbar.

## STUDY I

### Step 1: Stationary

- 1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 2 Select the **Modify model configuration for study step** checkbox.
- 3 In the tree, select **Component I (comp1) > Definitions > Variables for adjusting Vg to obtain specified drain current**.
- 4 Click  **Disable**.
- 5 In the tree, select **Component I (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 2**.
- 6 Click  **Disable**.
- 7 In the tree, select **Component I (comp1) > Electrostatics (electrolyte) (es) > Electric Displacement Field from semiconductor side**.
- 8 Click  **Disable**.
- 9 In the tree, select **Component I (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 2**.
- 10 Click  **Disable**.
- 11 In the tree, select **Component I (comp1) > Boundary ODE for oxide surface potential phiM (bode) > Initial Values 2**.
- 12 Click  **Disable**.
- 13 In the tree, select **Component I (comp1) > Global ODE to adjust Vg for specified drain current (ge2)**.
- 14 Click  **Disable in Model**.  
It is necessary to disable one of the global equations because they share the same dependent variable name (Vg).
- 15 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 16 Click  **Add**.


17 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
pHb (pH of bulk electrolyte)	range (3, 1, 11)	

18 In the **Model Builder** window, click **Study 1**.

19 In the **Settings** window for **Study**, type **Electrolyte** only in the **Label** text field.

20 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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

The result can be compared to the one from the 1D approximation formula. First evaluate a list of electrolyte potentials to plug into the 1D approximation formula.

## RESULTS

### *Point Evaluation 1*

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results > Derived Values** and choose **Point Evaluation**.

3 Select **Point 6** only.

4 In the **Settings** window for **Point Evaluation**, locate the **Expressions** section.

5 In the table, enter the following settings:

Expression	Unit	Description
phil-phil_bulk_g	V	Electrolyte potential to plug into 1D approximation formula

6 Click  **Evaluate**.

## TABLE 1

1 Go to the **Table 1** window.

2 Click the **Copy Table and Headers to Clipboard** button in the window toolbar.

Paste the table content into a text editor. Format the column of electrolyte potential values into a single line. Copy the line of electrolyte potential values to paste into the **Auxiliary Sweep** parameter table in the next study step (see below).

## ADD STUDY

1 Go to the **Add Study** window.








2 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Semiconductor (semi)**, **Electrostatics (electrolyte) (es)**,

**Transport of Charge Carriers (electrolyte) (tcc),  
Boundary ODE for oxide surface potential phiM (bode),  
Global ODE to copy specified Vg value (ge), and  
Global ODE to adjust Vg for specified drain current (ge2).**

- 3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Stationary**.
- 4 Click the **Add Study** button in the window toolbar.

## STUDY 2

### *Step 1: Stationary*

- 1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 2 Select the **Modify model configuration for study step** checkbox.
- 3 In the tree, select **Component 1 (comp1) > Definitions > Variables for adjusting Vg to obtain specified drain current**.
- 4 Click  **Disable**.
- 5 In the tree, select **Component 1 (comp1) > Definitions > Variables on oxide surface**.
- 6 Click  **Disable**.
- 7 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 2**.
- 8 Click  **Disable**.
- 9 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 2**.
- 10 Click  **Disable**.
- 11 In the tree, select **Component 1 (comp1) > Boundary ODE for oxide surface potential phiM (bode) > Initial Values 2**.
- 12 Click  **Disable**.
- 13 In the tree, select **Component 1 (comp1) > Global ODE to adjust Vg for specified drain current (ge2)**.
- 14 Click  **Disable in Model**.
- 15 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 16 Click  **Add**.

17 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
phi2_aprx (Potential at outer Helmholtz plane (control parameter for 1D approx.))		V

Now paste the line of electrolyte potential values into the **Auxiliary Sweep** parameter table, as shown below.

18 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
phi2_aprx (Potential at outer Helmholtz plane (control parameter for 1D approx.))	-9.084249078E-4 - 0.004637217778 - 0.01188430850 - 0.02083132004 - 0.03018603909 - 0.03930650544 - 0.04789552279 - 0.05583282929 - 0.06297207279	V

19 In the **Model Builder** window, click **Study 2**.

20 In the **Settings** window for **Study**, type 1D approx for electrolyte only in the **Label** text field.


21 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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

Now, create a plot to compare the 2D model result to the 1D approximation formula.

## RESULTS

*phi1: 2D Model vs. 1D Approx.*

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

2 In the **Settings** window for **ID Plot Group**, type phi1: 2D Model vs. 1D Approx. in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.


4 In the **Title** text area, type Electrolyte potential (V) - solid curves: 2D model, dotted curves: 1D approx..

*Line Graph: 2D model*

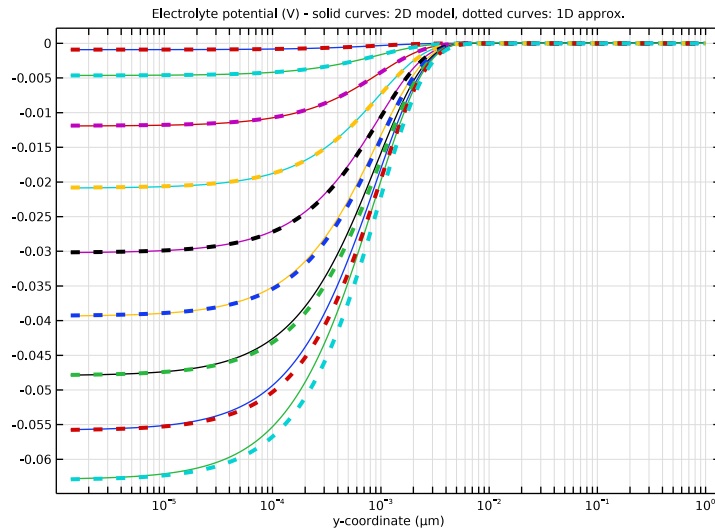
1 Right-click **phi1: 2D Model vs. 1D Approx.** and choose **Line Graph**.

- 2 In the **Settings** window for **Line Graph**, type Line Graph: 2D model in the **Label** text field.
- 3 Select Boundary 8 only.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type `phi1-phi1_bulk_g`.
- 5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 6 In the **Expression** text field, type `y`.

*Line Graph: 1D approx.*

- 1 Right-click **Line Graph: 2D model** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, type Line Graph: 1D approx. in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **1D approx for electrolyte only/ Solution 2 (sol2)**.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type `phi2_aprx*exp(-y/xD)`.
- 5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
- 6 From the **Width** list, choose **3**.
- 7 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

8 In the **phil: 2D Model vs. 1D Approx.** toolbar, click  **Plot**.



The 1D approximation reproduces the general trend of the electrolyte potential along the centerline of the electrolyte domain, as one would expect.

Next let us only look at the semiconductor, with the oxide surface potential provided by the solution of the electrolyte-only study.







#### ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Electrostatics (electrolyte) (es)**, **Transport of Charge Carriers (electrolyte) (tcc)**, **Boundary ODE for oxide surface potential phiM (bode)**, **Global ODE to copy specified Vg value (ge)**, and **Global ODE to adjust Vg for specified drain current (ge2)**.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Stationary**.
- 4 Click the **Add Study** button in the window toolbar.


#### STUDY 3

*Step 1: Stationary*

- 1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 2 Select the **Modify model configuration for study step** checkbox.

- 3 In the tree, select **Component 1 (comp1) > Definitions > Variables for adjusting Vg to obtain specified drain current.**
- 4 Click  **Disable.**
- 5 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 2.**
- 6 Click  **Disable.**
- 7 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 2.**
- 8 Click  **Disable.**
- 9 In the tree, select **Component 1 (comp1) > Boundary ODE for oxide surface potential phiM (bode) > Initial Values 2.**
- 10 Click  **Disable.**
- 11 In the tree, select **Component 1 (comp1) > Global ODE to adjust Vg for specified drain current (ge2).**
- 12 Click  **Disable in Model.**
- 13 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled.**
- 14 From the **Method** list, choose **Solution.**
- 15 From the **Study** list, choose **Electrolyte only, Stationary.**
- 16 From the **Parameter value (pHb)** list, choose **First.**
- 17 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 18 Click  **Add.**
- 19 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vd (Drain voltage)	0 10	mV






- 20 In the **Model Builder** window, click **Study 3.**
- 21 In the **Settings** window for **Study**, type Semiconductor only in the **Label** text field.
- 22 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.
- 23 In the **Study** toolbar, click  **Compute.**

You are now ready to solve the fully coupled model. First, fix the pH of the bulk electrolyte and sweep the gate voltage  $V_g$ . The result will demonstrate the concept that the electrolyte in the ISFET plays an analogous role as the gate contact in a MOSFET.

#### ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Global ODE to copy specified  $V_g$  value (ge)** and **Global ODE to adjust  $V_g$  for specified drain current (ge2)**.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Stationary**.
- 4 Click the **Add Study** button in the window toolbar.

#### SWEEP $V_g$ WITH CONSTANT PH



- 1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 2 Select the **Modify model configuration for study step** checkbox.
- 3 In the tree, select **Component 1 (comp1) > Definitions > Variables for adjusting  $V_g$  to obtain specified drain current**.
- 4 Click  **Disable**.
- 5 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 2**.
- 6 Click  **Disable**.
- 7 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 2**.
- 8 Click  **Disable**.
- 9 In the tree, select **Component 1 (comp1) > Boundary ODE for oxide surface potential  $\phi_{iM}$  (bode) > Initial Values 2**.
- 10 Click  **Disable**.
- 11 In the tree, select **Component 1 (comp1) > Global ODE to adjust  $V_g$  for specified drain current (ge2)**.
- 12 Click  **Disable in Model**.
- 13 Locate the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 14 From the **Method** list, choose **Solution**.
- 15 From the **Study** list, choose **Semiconductor only, Stationary**.

- 16 From the **Parameter value (Vd (mV))** list, choose **Last**.
- 17 Locate the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 18 Click **+ Add**.
- 19 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vga (Gate voltage (applied))	range (0, 0.2, 3)	V

- 20 In the **Model Builder** window, click **Study 4**.
- 21 In the **Settings** window for **Study**, type Sweep Vg with constant pH in the **Label** text field.
- 22 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.


*Solution 4 (sol4)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 4 (sol4)** node.
- 3 In the **Model Builder** window, expand the **Sweep Vg with constant pH > Solver Configurations > Solution 4 (sol4) > Stationary Solver 1** node, then click **Direct (Merged)**.
- 4 In the **Settings** window for **Direct**, click to expand the **Error** section.
- 5 Select the **Use in nonlinear solver** checkbox.  
This setting helps the convergence of highly nonlinear models.
- 6 In the **Study** toolbar, click  **Compute**.

Plot the drain current as a function of the gate voltage Vg.

**RESULTS**

*Id vs. Vg*


- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Id vs. Vg in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sweep Vg with constant pH/ Solution 4 (sol4)**.

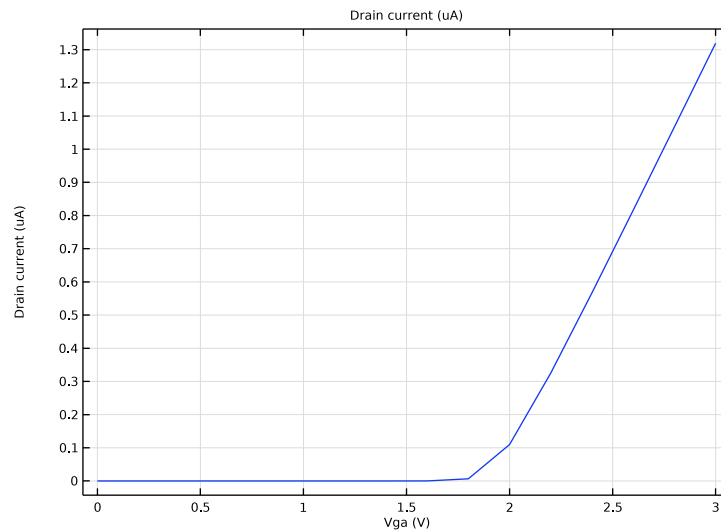
*Global I*

- 1 Right-click **Id vs. Vg** and choose **Global**.

- 2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Semiconductor > Terminals > semi.I0\_2 - Terminal current - A**.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
semi.I0_2	uA	Drain current

- 4 Click to expand the **Legends** section. Clear the **Show legends** checkbox.
- 5 In the **Id vs. Vg** toolbar, click  **Plot**.



The figure indeed shows the same  $I_d$ - $V_g$  behavior as one would observe in a typical MOSFET.

For the ISFET, the effective gate voltage is a function of both the applied voltage (as seen in the above figure), and the pH of the bulk electrolyte. To see this, fix the applied voltage  $V_g$  at some operating point, say, 2.6 V, that gives some nontrivial drain current. Then, sweep the pH value of the bulk electrolyte  $pH_b$ , and look at the behavior of the drain current versus drain voltage curve.

#### ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Find the **Studies** subsection. In the **Select Study** tree, select **Empty Study**.

3 Click the **Add Study** button in the window toolbar.

#### **SWEEP PH AND VD WITH FIXED VG**

1 In the **Settings** window for **Study**, type Sweep pH and Vd with fixed Vg in the **Label** text field.

2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

#### **SWEEP VG WITH CONSTANT PH**

*Step 1: Stationary*

In the **Model Builder** window, under **Sweep Vg with constant pH** right-click

**Step 1: Stationary** and choose **Copy**.

#### **SWEEP PH AND VD WITH FIXED VG**

In the **Model Builder** window, right-click **Sweep pH and Vd with fixed Vg** and choose **Paste Stationary**.

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

2 In the tree, select **Component 1 (comp1) > Global ODE to copy specified Vg value (ge)**.

3 Click  **Solve For**.


4 Locate the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Study** list, choose **Sweep Vg with constant pH, Stationary**.

5 From the **Parameter value (Vga (V))** list, choose **2.6 V**.

6 Locate the **Study Extensions** section. From the **Sweep type** list, choose **All combinations**.


7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vga (Gate voltage (applied))	2.6	V

8 Click  **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
pHb (pH of bulk electrolyte)	3 7 11	


10 Click  **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vd (Drain voltage)	range(0,0.2,1.2)^2	V

12 From the **Reuse solution from previous step** list, choose **Auto**.

*Solution 5 (sol5)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 5 (sol5)** node.
- 3 In the **Model Builder** window, expand the **Sweep pH and Vd with fixed Vg > Solver Configurations > Solution 5 (sol5) > Stationary Solver 1** node, then click **Direct (Merged)**.
- 4 In the **Settings** window for **Direct**, locate the **Error** section.
- 5 Select the **Use in nonlinear solver** checkbox.


This setting helps the convergence of highly nonlinear models.

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

Plot the drain current as a function of the drain voltage, for the 3 different pH values of the bulk electrolyte.

**RESULTS**

*Id-Vd curves for 3 different pH values*

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Id-Vd curves for 3 different pH values in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Sweep pH and Vd with fixed Vg/ Solution 5 (sol5)**.

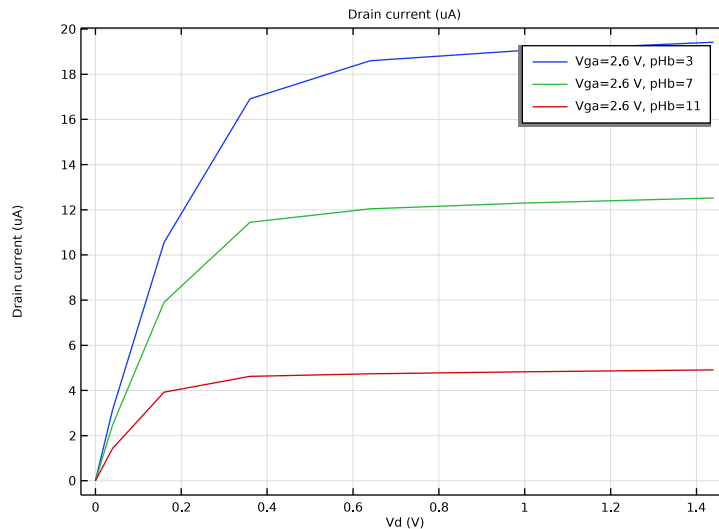
*Global I*

- 1 Right-click **Id-Vd curves for 3 different pH values** and choose **Global**.
- 2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Semiconductor > Terminals > semi.I0\_2 - Terminal current - A**.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
semi.I0_2	uA	Drain current

4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** checkbox.

5 In the **Id-Vd curves for 3 different pH values** toolbar, click  **Plot**.




Note that the Id-Vd curve of the ISFET is modulated by the pH value of the bulk electrolyte, in exact analogy to how the Id-Vd curve of a MOSFET is modulated by the gate voltage. In other words, the effective gate voltage seen by the ISFET is modulated by the pH value of the bulk electrolyte. This provides the basic sensing mechanism for measuring the pH value.

In a real device, a feedback circuit adjusts the gate voltage for a given electrolyte, such that the drain current is maintained at a constant set point. In other words, the applied gate voltage is used to compensate for the effect of the pH. Thus in this case the applied gate voltage becomes the indicator for the pH value. You can simulate this mode of operation using a global equation, without having to model the details of the feedback circuit.

Arbitrarily choose the operating point at the drain voltage of 1 V and drain current of 18 uA, which is close to the values given by the Id-Vd curve for the pH value of 3 (see graph above). In the next study, you will sweep the pH value from 3 up to 11, using the solution from the previous study as the initial condition. Note that the global equation in the previous study made a copy of the applied gate voltage, in order to provide the initial condition for the other global equation in the next study.

#### ADD STUDY

1 Go to the **Add Study** window.

- 2 Find the **Studies** subsection. In the **Select Study** tree, select **Empty Study**.
- 3 Click the **Add Study** button in the window toolbar.
- 4 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

#### **SWEEP PH WITH FIXED ID**

- 1 In the **Settings** window for **Study**, type Sweep pH with fixed Id in the **Label** text field.
- 2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

Toggle off the **Add Study** window.

#### **SWEEP PH AND VD WITH FIXED VG**






*Step 1: Stationary*






In the **Model Builder** window, under **Sweep pH and Vd with fixed Vg** right-click

**Step 1: Stationary** and choose **Copy**.


#### **SWEEP PH WITH FIXED ID**

In the **Model Builder** window, right-click **Sweep pH with fixed Id** and choose **Paste Stationary**.

- 1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 2 In the tree, select **Component 1 (comp1) > Definitions > Variables for applying specified gate voltage (Vg)**.
- 3 Click  **Disable**.
- 4 In the tree, select **Component 1 (comp1) > Definitions > Variables for adjusting Vg to obtain specified drain current**.
- 5 Click  **Enable**.
- 6 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 1**.
- 7 Click  **Disable**.
- 8 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Electric Potential 2**.
- 9 Click  **Enable**.
- 10 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 1**.
- 11 Click  **Disable**.

- 12 In the tree, select **Component 1 (comp1) > Electrostatics (electrolyte) (es) > Surface Charge Density 2**.
- 13 Click  **Enable**.
- 14 In the tree, select **Component 1 (comp1) > Boundary ODE for oxide surface potential phiM (bode) > Initial Values 2**.
- 15 Click  **Enable**.
- 16 In the tree, select **Component 1 (comp1) > Global ODE to copy specified Vg value (ge)**.
- 17 Click  **Disable in Model**.
- 18 In the tree, select **Component 1 (comp1) > Global ODE to adjust Vg for specified drain current (ge2)**.
- 19 Click  **Solve For**.
- 20 Locate the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Study** list, choose **Sweep pH and Vd with fixed Vg, Stationary**.
- 21 From the **Parameter value (Vd (V),Vga (V),pHb)** list, choose **6: Vd=1 V, Vga=2.6 V, pHb=3**.
- 22 Locate the **Study Extensions** section. Click to select row number 1 in the table.
- 23 Click  **Delete**.
- 24 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
pHb (pH of bulk electrolyte)	3 5 7 9 11	

- 25 Click  **Move Down**.
- 26 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vd (Drain voltage)	1	V

- 27 From the **Run continuation for** list, choose **No parameter**.
- 28 From the **Reuse solution from previous step** list, choose **Yes**.


*Solution 6 (sol6)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 6 (sol6)** node.
- 3 In the **Model Builder** window, expand the **Sweep pH with fixed Id > Solver Configurations > Solution 6 (sol6) > Stationary Solver 1** node, then click **Direct (Merged)**.

4 In the **Settings** window for **Direct**, locate the **Error** section.

5 Select the **Use in nonlinear solver** checkbox.


This setting helps the convergence of highly nonlinear models.

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

Now, plot the gate voltage versus the pH of the bulk electrolyte. This is the sensitivity curve of the ISFET, since the pH is the input and the gate voltage is the output of the pH sensor.

## RESULTS

*Vg vs. pH - sensitivity curve of the ISFET*

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

2 In the **Settings** window for **ID Plot Group**, type Vg vs. pH - sensitivity curve of the ISFET in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Sweep pH with fixed Id/ Solution 6 (sol6)**.

4 Locate the **Legend** section. Clear the **Show legends** checkbox.

*Global 1*

1 Right-click **Vg vs. pH - sensitivity curve of the ISFET** and choose **Global**.


2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

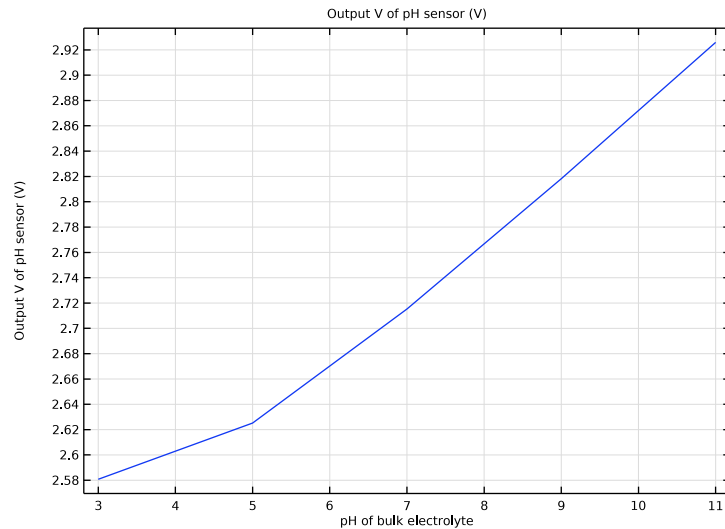
3 In the table, enter the following settings:

Expression	Unit	Description
Vg	V	Output V of pH sensor

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

5 In the **Expression** text field, type pHb.


6 In the **Vg vs. pH - sensitivity curve of the ISFET** toolbar, click  **Plot**.



The sensitivity of the ISFET is given by the slope of the curve. The result is consistent with the one reported in the reference paper.

Make a colorful plot of the electric potential for the model thumbnail.

#### 2D Plot Group 5


- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Sweep pH with fixed Id/Solution 6 (sol6)**.
- 4 From the **Parameter value (pHb)** list, choose **3**.

#### Surface 1

Right-click **2D Plot Group 5** and choose **Surface**.

#### Surface 2

- 1 In the **Model Builder** window, right-click **Surface 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type  $V$ .
- 4 Click to expand the **Quality** section. From the **Evaluation settings** list, choose **Manual**.
- 5 From the **Resolution** list, choose **No refinement**.
- 6 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

7 In the **2D Plot Group 5** toolbar, click  **Plot**.

