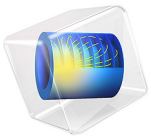
Created in COMSOL Multiphysics 6.1



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

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

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 physics involved in the semiconductor domain are similar to those in the MOSFET tutorial in the Application Libraries. The physics for the electrolyte domain are similar to those in the Diffuse Double Layer tutorial. Users are encouraged to familiarize themselves with those two tutorials first.

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, 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

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.

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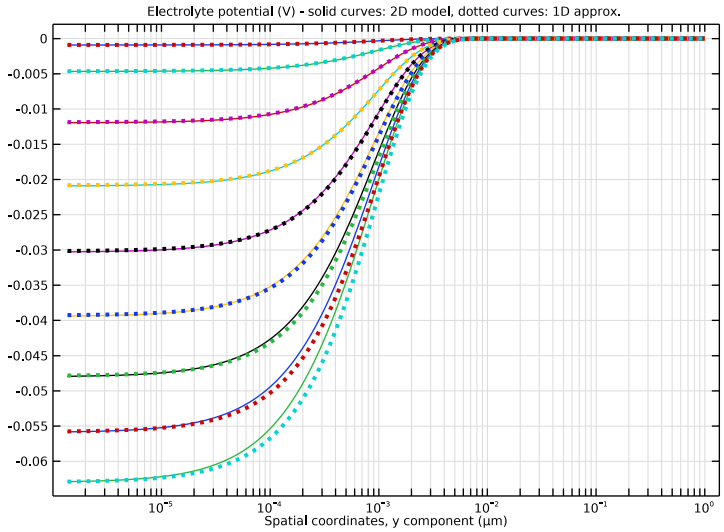


Figure 1: Electrolyte potential along the centerline of the electrolyte domain. (It does not extrapolate to the dielectric surface potential at y=0 because the voltage drop across the Stern layer is not explicitly modeled in the electrolyte domain. See Model Definition *for details.)*

Figure 2 shows the drain current as a function of the gate voltage for the fully coupled system. The behavior of this Id-Vg 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.

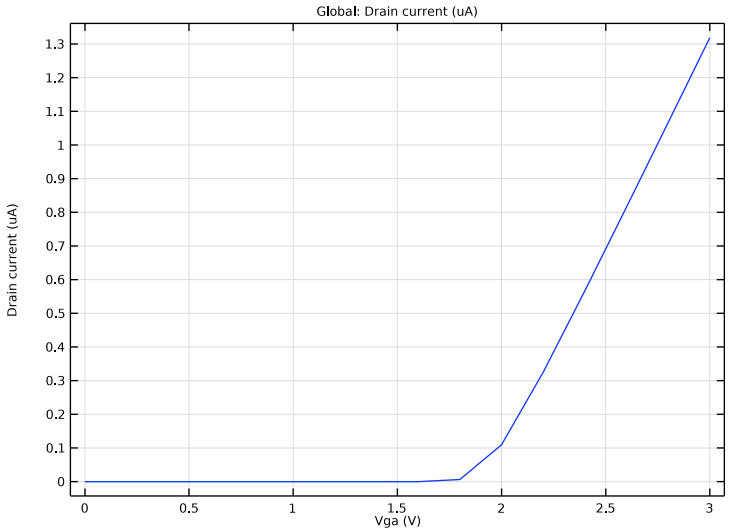


Figure 2: Drain current as a function of the applied gate voltage.

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.

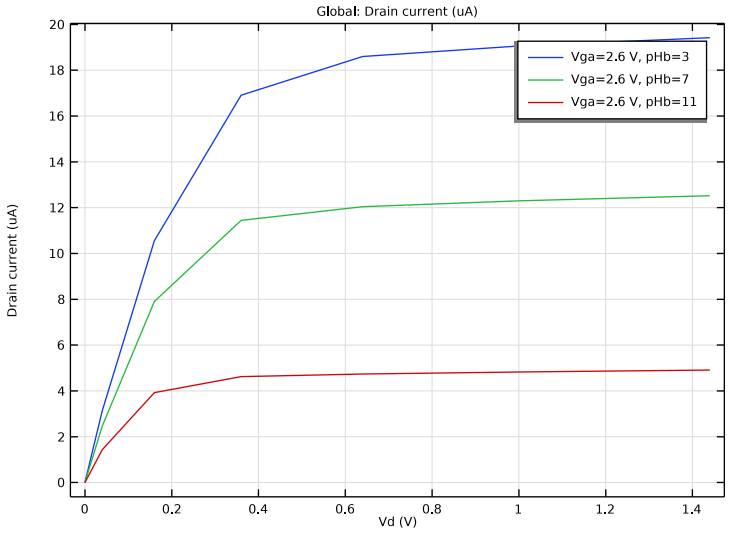


Figure 3: Drain current - drain voltage curves for three different pH values.

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.

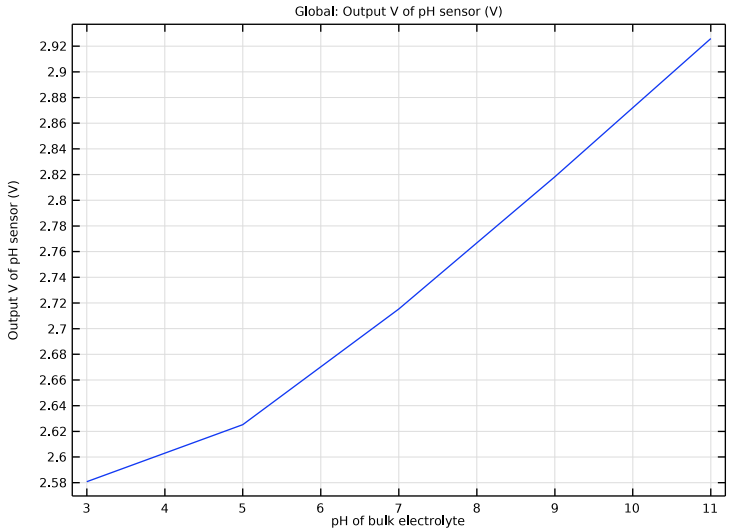


Figure 4: Sensitivity curve for the ISFET pH sensor.

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://www.sciencedirect.com/science/article/pii/S0001868696003077)

Application Library path: `Semiconductor_Module/Photonic_Devices_and_Sensors/isfet`

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 1

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.txt`.

Next build the geometric objects in the model.

GEOMETRY 1

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 (µm)	y (µm)
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 (µm)	y (µm)
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:

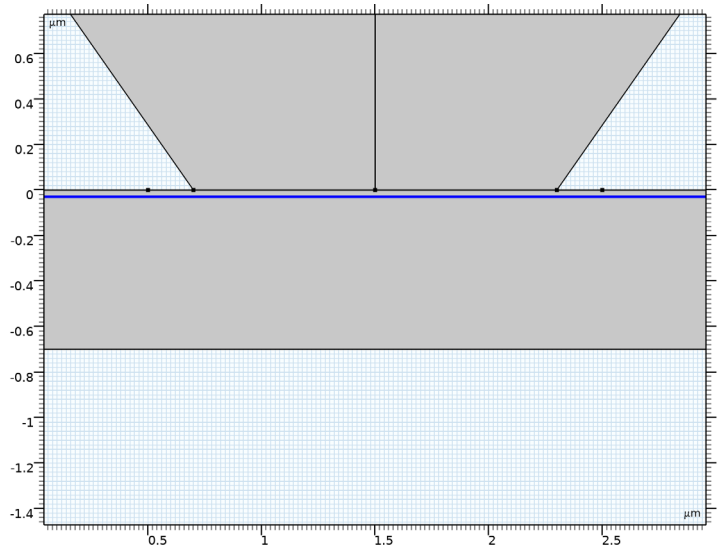
x (µm)	y (µm)
1.5	0
1.5	1

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 (Vg)

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 (Vg)` in the **Label** text field.

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

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

Variables for adjusting Vg to obtain specified drain current

1 Right-click **Variables for applying specified gate voltage (Vg)** and choose **Duplicate**.

2 In the **Settings** window for **Variables**, type `Variables for adjusting Vg 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	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	cH_bulk*exp(-(phiM-phil_bulk)/V_therm)		Activity of H+
rhos0	e_const*Ns*(aHs^2-Ka*Kb)/(Ka*Kb+Kb*aHs+aHs^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 **Add to Component** 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 box, 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	epsilonr_iso ; epsilonrii = epsilonr_iso, epsilonrij = 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

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** check box.

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

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 `Vd`.

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 `phiM`.

5 Locate the **Gate Contact** section. In the ε_{ins} text field, type `4.5`.

6 In the d_{ins} text field, type `30[nm]`.

7 In the Φ text field, type `0[V]`.

The undefined variable `phiM` will be defined later.

Now set up the physics for the electrolyte, similar to the Diffuse Double Layer tutorial in the Application Libraries.

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** text field, type `phi`.

5 Click **Add to Component 1** 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 **Chemical Species Transport>Transport of Diluted Species (tds)**.

3 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type `4`.

4 In the **Concentrations** table, enter the following settings:

cA
cX
cH
cOH

5 Click **Add to Component 1** in the window toolbar.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Settings** window for **Transport of Diluted Species**, 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 **Mathematics>ODE and DAE Interfaces>Boundary ODEs and DAEs (bode)**.

3 Click to expand the **Dependent Variables** section. In the **Dependent variables** table, enter the following settings:

phiM

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

ADD PHYSICS

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

2 In the tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.

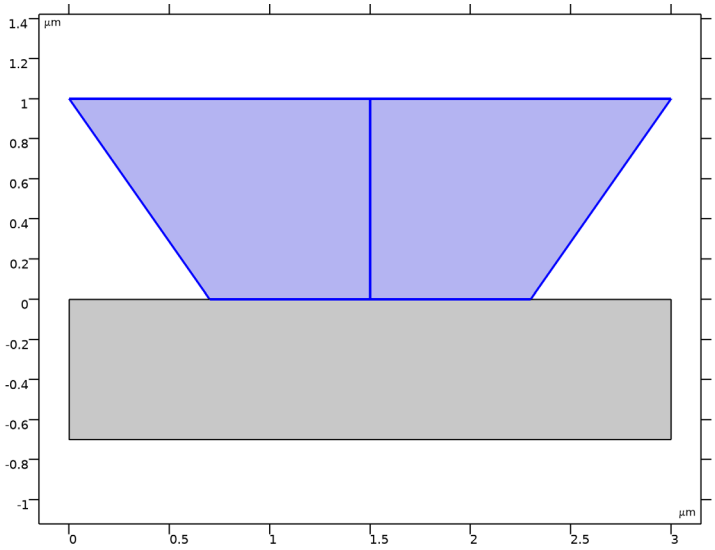
3 Click **Add to Component 1** in the window toolbar.

4 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

ELECTROSTATICS (ELECTROLYTE)

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

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



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

TRANSPORT OF DILUTED SPECIES (ELECTROLYTE)

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

2 In the **Settings** window for **Transport of Diluted Species**, type `Transport of Diluted Species (electrolyte)` in the **Label** text field.

3 Locate the **Transport Mechanisms** section. Clear the **Convection** check box.

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

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

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 phiM` in the **Label** text field.

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

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

5 Click **Filter**.

6 In the tree, select **Electromagnetics>Electric potential (V)**.

7 Click **OK**.

8 In the **Settings** window for **Boundary ODEs and DAEs**, locate the **Units** section.

9 Click **Select Source Term Quantity**.

10 In the **Physical Quantity** dialog box, click **Filter**.

11 In the tree, select **Electromagnetics>Electric potential (V)**.

12 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.

MULTIPHYSICS

Potential Coupling 1 (pc1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Multiphysics** and choose **Potential Coupling**.

2 In the **Settings** window for **Potential Coupling**, locate the **Domain Selection** section.

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

Note that the software determines the coupled physics interfaces automatically, and only allows the multiphysics coupling in relevant domains.

Space Charge Density Coupling 1 (scdc1)

1 In the **Model Builder** window, right-click **Multiphysics** and choose **Space Charge Density Coupling**.

2 In the **Settings** window for **Space Charge Density Coupling**, locate the **Domain Selection** section.

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

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`.

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

`semi.nD_ins*semi.nX`	`x`
`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 ρ_s text field, type `rhos0`.

Set up the transport physics for the electrolyte.

Species Charges

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

2 In the **Settings** window for **Species Properties**, locate the **Charge** section.

3 In the z_{cA} text field, type `zA`.

4 In the z_{cX} text field, type `zX`.

5 In the z_{cH} text field, type `1`.

6 In the z_{cOH} text field, type `-1`.

Transport Properties 1

1 In the **Model Builder** window, click **Transport Properties 1**.

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

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

4 Locate the **Diffusion** section. In the D_{cA} text field, type `DA`.

5 In the D_{cX} text field, type `DX`.

6 In the D_{cH} text field, type `DH`.

7 In the D_{cOH} text field, type `DOH`.

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 cA text field, type `cA_bulk`.

4 In the cX text field, type `cX_bulk`.

5 In the cH text field, type `cH_bulk`.

6 In the cOH text field, type `cOH_bulk`.

Concentration 1

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

2 Select Boundaries 5 and 10 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

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

5 In the $c_{0,cA}$ text field, type `cA_bulk`.

6 Select the **Species cX** check box.

7 In the $c_{0,cX}$ text field, type `cX_bulk`.

8 Select the **Species cH** check box.

9 In the $c_{0,cH}$ text field, type `cH_bulk`.

10 Select the **Species cOH** check box.

11 In the $c_{0,cOH}$ text field, type `cOH_bulk`.

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 PHIM (BODE)

Distributed ODE 1

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Boundary ODE for oxide surface potential phiM (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 `phil+es.nD/Ci_st-phiM`.

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 *phiM* text field, type `phil_bulk-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

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Global ODE to copy specified Vg value (ge)** click **Global Equations 1**.

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) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/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 box, click **Filter**.

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

1 In the **Model Builder** window, under **Component 1 (comp1)>Global ODE to adjust Vg for specified drain current (ge2)** click **Global Equations 1**.

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

3 Click **Select Dependent Variable Quantity**.

4 In the **Physical Quantity** dialog box, click **Filter**.

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) (1)	Initial value (u_0) (V)	Initial value (u_t0) (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** check box. In the associated text field, type `1.05`.

Size 2

In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Size 2** and choose **Delete**.

Size 3

In the **Model Builder** window, right-click **Size 3** and choose **Delete**.

Free Triangular 1

In the **Model Builder** window, right-click **Free Triangular 1** and choose **Delete**.

Edge 1

1 In the **Mesh** toolbar, click  **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 Clear the **Smooth across removed control entities** check box.

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** check box. 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. Clear the **Smooth across removed control entities** check box.

6 Click to expand the **Reduce Element Skewness** section. Select the **Adjust edge mesh** check box.

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** check box.

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. Clear the **Smooth across removed control entities** check box.

Boundary Layers 1

1 In the **Mesh** toolbar, click  **Boundary Layers**.

2 In the **Settings** window for **Boundary Layers**, locate the **Domain Selection** section.

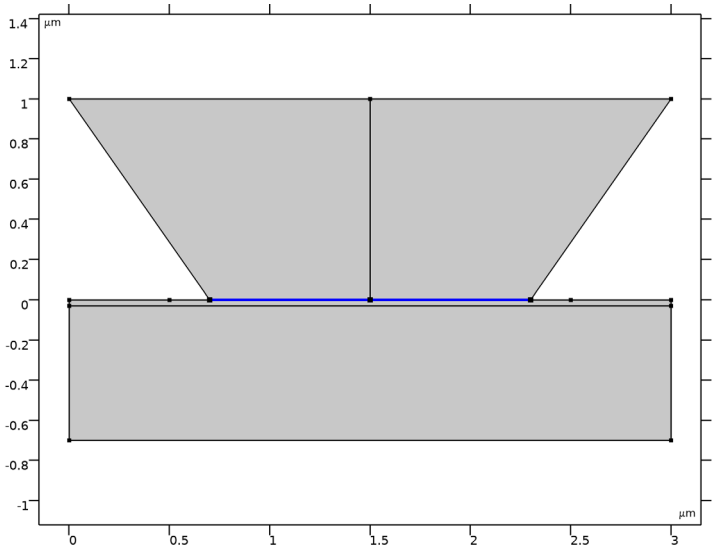
3 From the **Geometric entity level** list, choose **Domain**.

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** check boxes 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 **Add Study** in the window toolbar.

STUDY 1

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** check box.

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 Displacement Field from semiconductor side**.

6 Click **Disable**.

7 In the tree, select **Component 1 (comp1)> Global ODE to adjust Vg for specified drain current (ge2)**.

8 Click **Disable in Model**.

It is necessary to disable one of the global equations because they share the same dependent variable name (`Vg`).

9 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

10 Click **Add**.

11 In the table, enter the following settings:

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

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

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

14 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

15 In the **Home** 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	V	Electrolyte potential to plug into 1D approximation formula

6 Click **Evaluate**.

TABLE

1 Go to the **Table** window.

2 Click **Copy Table and Headers to Clipboard** 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** check boxes for **Semiconductor (semi)**, **Electrostatics (electrolyte) (es)**, **Transport of Diluted Species (electrolyte) (tds)**, **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 **Multiphysics couplings in study** subsection. In the table, clear the **Solve** check boxes for **Potential Coupling 1 (pc1)** and **Space Charge Density Coupling 1 (scdc1)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Stationary**.

5 Click **Add Study** 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** check box.

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)>Global ODE to adjust Vg for specified drain current (ge2)**.

8 Click **Disable in Model**.

9 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

10 Click **Add**.

11 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.

12 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

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

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

15 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

16 In the **Home** toolbar, click **Compute**.

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

RESULTS

phil: 2D Model vs. 1D Approx.

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `phil: 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.`.

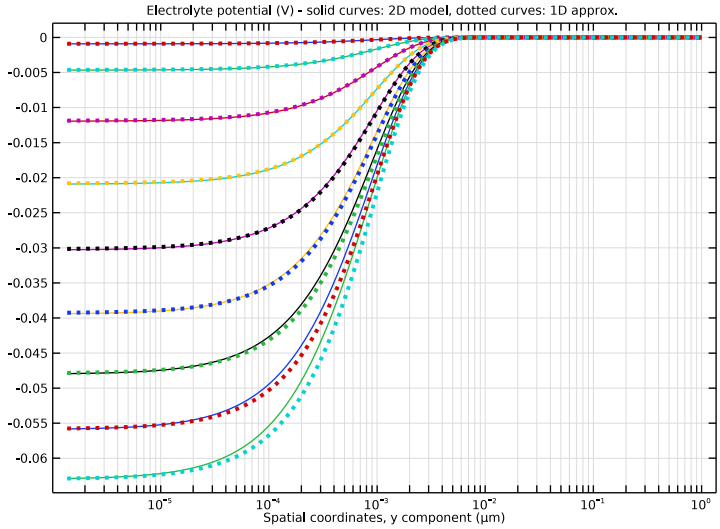
Line Graph: 2D model

1. Right-click **phil: 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 `phil-phil_bulk`.
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** check boxes for **Electrostatics (electrolyte) (es)**, **Transport of Diluted Species (electrolyte) (tds)**, **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 **Multiphysics couplings in study** subsection. In the table, clear the **Solve** check boxes for **Potential Coupling 1 (pc1)** and **Space Charge Density Coupling 1 (scdc1)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

5 Click **Add Study** 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** check box.

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)> Global ODE to adjust Vg for specified drain current (ge2)**.

6 Click **Disable in Model**.

7 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**.

8 From the **Method** list, choose **Solution**.

9 From the **Study** list, choose **Electrolyte only, Stationary**.

10 From the **Parameter value (pHb)** list, choose **First**.

11 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

12 Click **Add**.

13 In the table, enter the following settings:

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

14 In the **Model Builder** window, click **Study 3**.

15 In the **Settings** window for **Study**, type `Semiconductor only` in the **Label** text field.

16 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

17 In the **Home** 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 `Vg`. 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** check boxes for **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 **Add Study** in the window toolbar.

STUDY 4

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** check box.

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)> Global ODE to adjust Vg for specified drain current (ge2)**.

6 Click **Disable in Model**.

7 Locate the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

8 From the **Method** list, choose **Solution**.

9 From the **Study** list, choose **Semiconductor only, Stationary**.

10 From the **Parameter value (Vd (mV))** list, choose **Last**.

11 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

12 Click **Add**.

13 In the table, enter the following settings:

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

14 In the **Model Builder** window, click **Study 4**.

15 In the **Settings** window for **Study**, type `Sweep Vg with constant pH` in the **Label** text field.

16 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

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** check box.

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

2 In the **Settings** window for **1D 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 1

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

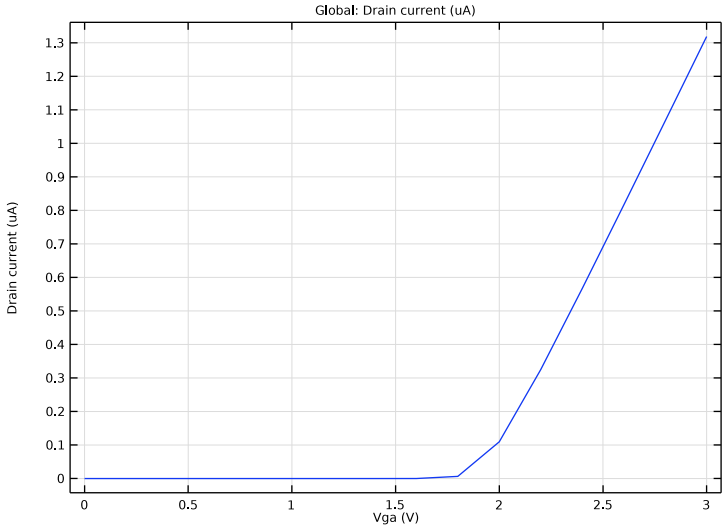
2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor> Terminals>semi.I0_2 - Terminal current - A**.

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** check box.

5 In the **Id vs. Vg** toolbar, click **Plot**.



The figure indeed shows the same Id-Vg 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 `Vg` at some operating point, say, 2.6 V, that gives some nontrivial drain current. Then, sweep the pH value of the bulk electrolyte `pHb`, 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 **Add Study** 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** check box.

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**.

Step 1: 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** check box.

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

2 In the **Settings** window for **1D 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 1

1 Right-click **Id-Vd curves for 3 different pH values** and choose **Global**.

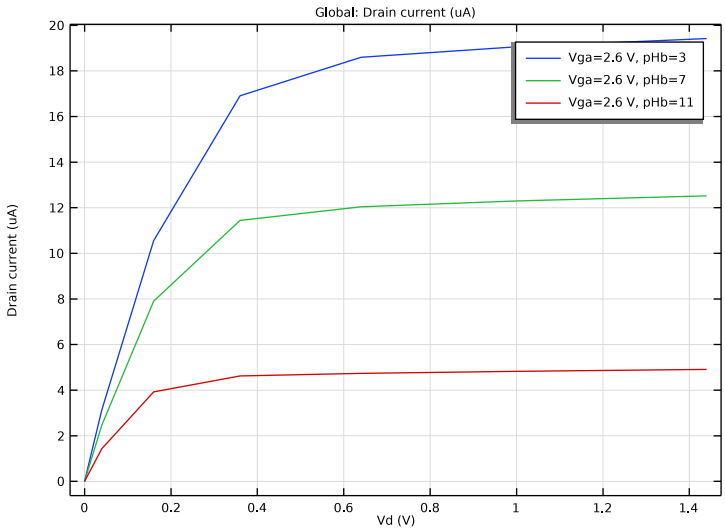
2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Semiconductor> Terminals>semi.I0_2 - Terminal current - A**.

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** check box.

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 **Add Study** 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** check box.

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**.

Step 1: 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)>Global ODE to copy specified Vg value (ge)**.

7 Click **Disable in Model**.

8 In the tree, select **Component 1 (comp1)> Global ODE to adjust Vg for specified drain current (ge2)**.

9 Click **Solve For**.

10 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**.

11 From the **Parameter value (Vd (V),Vga (V),pHb)** list, choose **6: Vd=1 V, Vga=2.6 V, pHb=3**.

12 Locate the **Study Extensions** section. Click to select row number 1 in the table.

13 Click **Delete**.

14 In the table, enter the following settings:

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

15 Click **Move Down**.

16 In the table, enter the following settings:

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

17 From the **Run continuation for** list, choose **No parameter**.

18 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** check box.

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

2 In the **Settings** window for **1D 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** check box.

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.

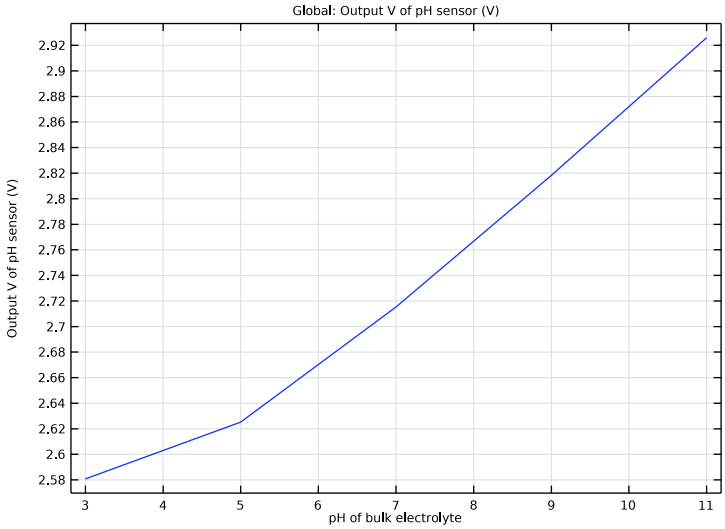
3 In the table, enter the following settings:

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 **Home** toolbar, click **Add Plot Group** and choose **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 **Resolution** list, choose **No refinement**.
5. Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.
6. In the **2D Plot Group 5** toolbar, click **Plot**.