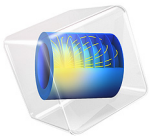
Created in COMSOL Multiphysics 6.2



Density-Gradient Analysis of an InSb p-Channel FET

This tutorial analyzes the DC characteristics of an InSb p-Channel FET, using the density-gradient theory to add the effect of quantum confinement to the conventional drift–diffusion formulation, without a large increase of computational resources. The confinement effect is applied both in the quantum well channel and on the top insulator interface, which is close to the channel. The use of an anisotropic density-gradient effective mass matrix is demonstrated, as is the technique to configure a general field-dependent mobility model. The hole density profile and the Id–Vg curve obtained from the 2D model compare well with the published figures in the reference paper.

Introduction

As the semiconductor fabrication technology progresses to produce smaller and smaller devices, the effect of quantum confinement becomes more and more important. This tutorial follows the approach described in Ref. 1 to compute the hole density distribution and drain current as a function of the gate voltage of an InSb p-channel FET using the density-gradient theory (as reviewed in Ref. 2).

Model Definition

The model computes the hole density profile at pinch-off and the drain characteristics of an InSb p-channel FET, to be compared with Fig. 7 and 8 in Ref. 1. Not all simulation details are given in the paper. Nevertheless, the approach described in the paper is followed as closely as possible. When a parameter is not listed, a typical value found in the literature is used in the model: some of the material properties of InSb are taken from Ref. 3. The lead author of Ref. 1, Dr. Ancona, has also kindly verified that the Schottky barrier should be 0.4 eV and the Be delta doping is 2 nm thick with concentration $1{\cdot}10^{19}$ cm^{-3} (private communication). The section Modeling Instructions lists all the parameters used in the model.

The channel of the simulated structure is formed by a 5 nm thick InSb quantum well layer built on top of an AlInSb barrier bulk material. A 10 nm thick barrier layer is then added on top of the quantum well layer, followed by the p+ caps for the source and drain contacts. (See Fig. 6 in Ref. 1, though the gate is not recessed in this model.)

The quantum confinement effect for the quantum well layer is automatically accounted for with the default **Continuous quasi-Fermi levels** option for the **Continuity/Heterojunction** boundary condition, active at the well–barrier interfaces. In addition, quantum confinement effect for the top barrier layer boundary (the top barrier–vacuum interface) is added by selecting the **Potential barrier** option for the **Insulation** boundary condition

active at those boundaries. The temperature is assumed to be 300 K. Fermi–Dirac statistics is used.

The density-gradient effective mass is anisotropic in this model. This is done by selecting the **Diagonal** option under the section **Material Properties, Density-Gradient** in the settings window for the **Semiconductor Material Model** domain condition.

A field dependent mobility model is employed by the reference paper. Even though it is sufficient to use the X-component of the electric field for the mobility model, given the simple geometry, we opt for the more general procedure, applicable to any arbitrary geometry. A **Caughey–Thomas Mobility Model (E)** subnode is added to the **Semiconductor Material Model** domain condition to provide the parallel component of the electric field to be used by the mobility model. The solver sequence is adjusted to achieve convergence for the resulting highly coupled system.

See the comments in the section Modeling Instructions for more detailed discussions on the model construction, meshing techniques, solution processes, and result visualization.

Results and Discussion

Figure 1 shows the drain current as a function of the gate voltage, to compare with Fig. 8 in Ref. 1. The general trend and threshold voltage compare well, with some minor differences in the magnitude of the current.

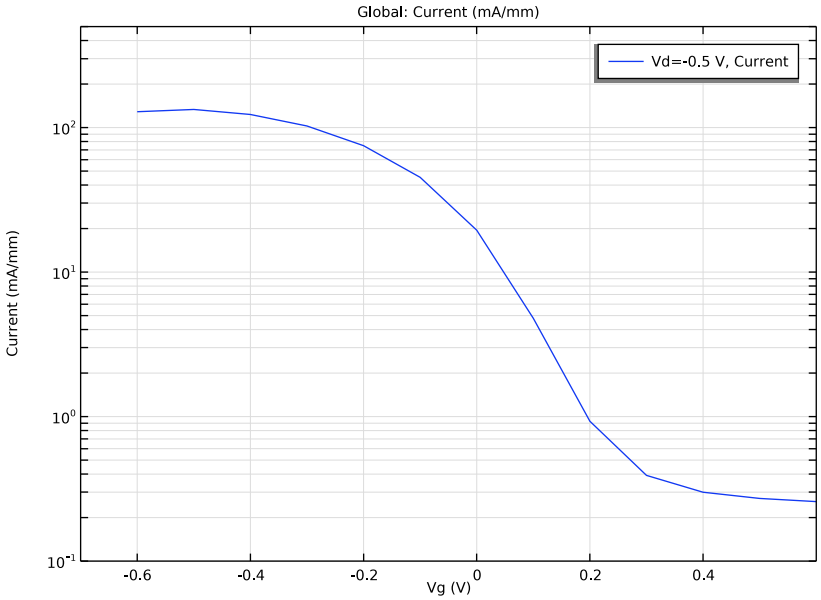


Figure 1: Drain current versus gate voltage curve.

Figure 2 plots the hole concentration profile at pinch-off, to compare with Fig. 7 in the reference paper. The overall agreement is quite good, with some small differences.

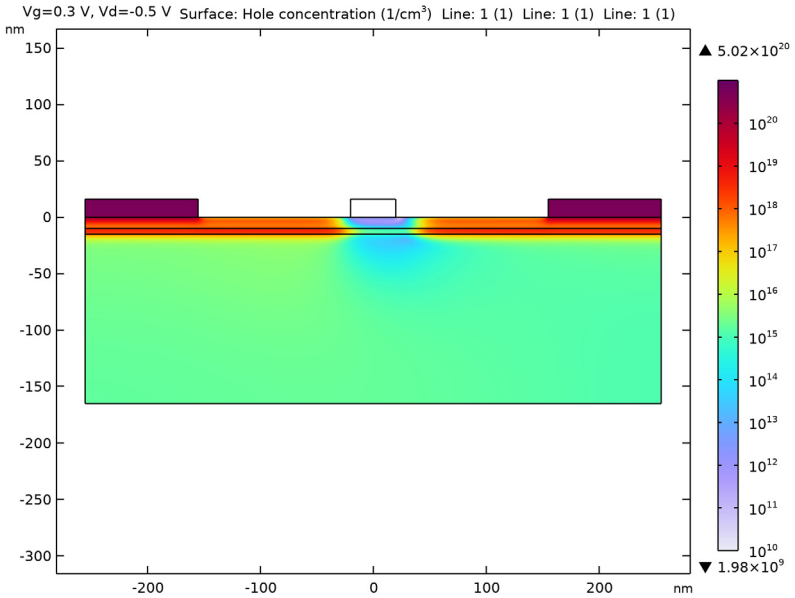


Figure 2: Hole concentration profile at pinch-off.

Figure 3 compares a line cut of the hole density profile at $x = -100$ nm with an approximate drift–diffusion profile, to show qualitatively the effect of quantum confinement both in the quantum well layer and at the top barrier–vacuum interface ($y = 0$ nm). The valence band edge and the quasi-Fermi level for the holes are also plotted. Note that this comparison is only qualitative, since the model is not re-solved using the conventional drift–diffusion formulation. As such, only the *shape* of the approximate drift–diffusion profile is representative of the result if the model was to be re-solved, and the absolute *magnitude* is not. Nevertheless the qualitative difference between the treatments with and without quantum confinement is well characterized by the difference in the *shape* of the hole concentration profiles: the lack of carrier pile-up at the heterojunctions and the

repulsion of carriers from the top barrier–vacuum interface are both clearly indicative of quantum confinement effects.

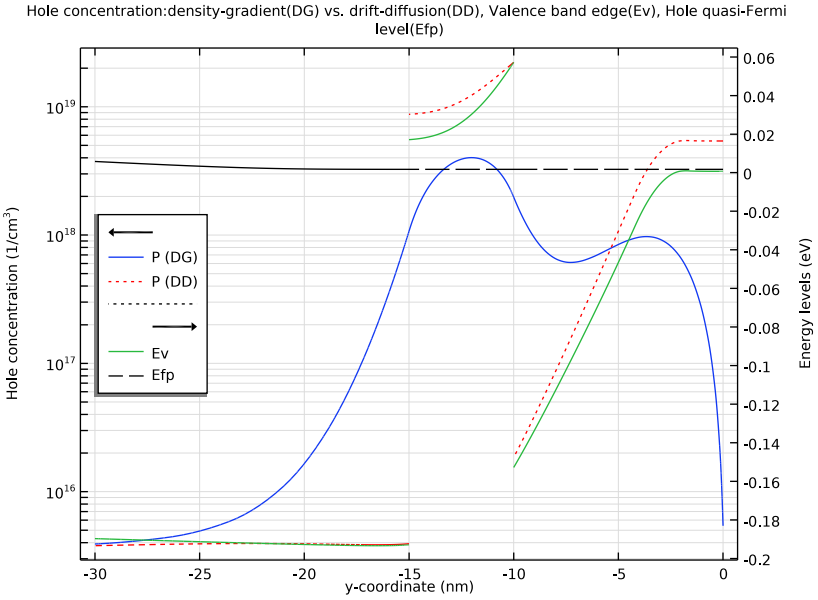


Figure 3: Hole concentration: density-gradient (DG) versus drift–diffusion (DD), valence band edge (Ev), and quasi-Fermi level for holes (Efp).

References

1. M.G. Ancona, B.R. Bennett, and J.B. Boos, "Scaling projections for Sb-based p-channel FETs," *Solid-State Electronics*, vol. 54, p. 1349, 2010.

2. M.G. Ancona, "Density-gradient theory: a macroscopic approach to quantum confinement and tunneling in semiconductor devices," *J. Comput. Electron.*, vol. 10, p. 65, 2011.

3. M. Levinshtein, S. Rumyantsev, and M. Shur, *Handbook Series on Semiconductor Parameters*, vol. 1, World Scientific, 1996, reprinted 2000.

Application Library path: `Semiconductor_Module/Transistors/insb_pfet_density_gradient`

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 **Study**.

The **Semiconductor Equilibrium** study step is suitable either to solve for systems known to be in thermal equilibrium, or, in this case, to provide a good initial condition for bias voltage sweeps starting from the equilibrium position.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Semiconductor Equilibrium**.

6 Click **Done**.

GEOMETRY 1

The Model Wizard starts the COMSOL Desktop at the **Geometry** node. Use this chance to select a convenient length unit. Then enter some dimensional parameters for building the geometry.

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 **nm**.

GLOBAL DEFINITIONS

Parameters 1: Geometry

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Parameters 1: Geometry` in the **Label** text field.

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

Name	Expression	Value	Description
Lgate	40[nm]	4E-8 m	Gate length
Lgate2cap	135[nm]	1.35E-7 m	Gate to cap length
Lcap	100[nm]	1E-7 m	Cap length
Hcap	16[nm]	1.6E-8 m	Cap height
Htopbar	10[nm]	1E-8 m	Top barrier height
Hwell	5[nm]	5E-9 m	Well height
Hbotbar	150[nm]	1.5E-7 m	Bottom barrier height
Hstack	Htopbar+Hwell+Hbotbar	1.65E-7 m	Total height
Ltot	Lgate+2*(Lgate2cap+Lcap)	5.1E-7 m	Total length
d0	1[um]	1E-6 m	Out-of-plane thickness

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 `Ltot`.

4 In the **Height** text field, type `Hstack`.

5 Locate the **Position** section. In the **x** text field, type `-Ltot/2`.

6 In the **y** text field, type `-Hstack`.

7 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (nm)
Layer 1	Hbotbar
Layer 2	Hwell

Rectangle 2 (r2)

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 `Ltot`.

4 In the **Height** text field, type `Hcap`.

5 Locate the **Position** section. In the **x** text field, type `-Ltot/2`.

6 Locate the **Layers** section. Clear the **Layers on bottom** check box.

7 Select the **Layers to the left** check box.

8 Select the **Layers to the right** check box.

9 In the table, enter the following settings:

Layer name	Thickness (nm)
`Layer 1`	`Lcap`
`Layer 2`	`Lgate2cap`

Delete Entities 1 (del1)

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Delete Entities**.

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

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

4 On the object **r2**, select Domains 2 and 4 only.

Enter some material parameters and then use the built-in silicon material as a template to apply the material data. Parameters not found in the reference paper are taken from volume 1 of Handbook Series on Semiconductor Parameters edited by Levinshtein, Rumyantsev, and Shur (1996, reprinted 2000). The electron affinity of the barrier is calculated to give the value of the valence band offset given in the reference paper. Use the continuation parameter to prepare for the ramp up of the band offsets from small values in order to achieve better convergence.

GLOBAL DEFINITIONS

Parameters 2: Materials

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters 2: Materials` in the **Label** text field.

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

Name	Expression	Value	Description
cp	1	1	Continuation parameter for heterojunction and doping
EgW0	0.17[V]	0.17 V	Band gap, well
EgB	0.78[V]	0.78 V	Band gap, barrier
deltaEv	0.21[V]	0.21 V	Valence band offset
chiW0	4.59[V]	4.59 V	Electron affinity, well
chiB	chiW0+EgW0+deltaEv-EgB	4.19 V	Electron affinity, barrier
EgW	EgW0*cp+EgB*(1-cp)	0.17 V	Band gap, well
chiW	chiW0*cp+chiB*(1-cp)	4.59 V	Electron affinity, well
epsrW	17.7	17.7	Dielectric constant, well
epsrB	15.7	15.7	Dielectric constant, barrier
PhiB	0.4[V]	0.4 V	Schottky barrier
Nv0	7.3e18[cm^-3]	7.3E24 1/m³	Effective valence band density of states
Nc0	4.2e16[cm^-3]	4.2E22 1/m³	Effective conduction band density of states
muLFW	1230[cm^2/V/s]	0.123 m²/(V·s)	LF hole mobility, well
muLFB	50[cm^2/V/s]	0.005 m²/(V·s)	LF hole mobility, barrier
vSat	8e6[cm/s]	80000 m/s	Saturation velocity
muSS	100[cm^2/V/s]	0.01 m²/(V·s)	SS hole mobility, all materials
ESS	3e5[V/cm]	3E7 V/m	SS electric field, all materials
mun0	7.7e4[cm^2/V/s]	7.7 m²/(V·s)	Electron mobility

Name	Expression	Value	Description
mpDGperp	0.04*me_const	3.6438E-32 kg	DG effective mass, perpendicular
mpDGpara	0.053*me_const	4.828E-32 kg	DG effective mass, parallel

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

InSb Well

1 In the **Settings** window for **Material**, type `InSb Well` in the **Label** text field.

2 Locate the **Geometric Entity Selection** section. Click **Clear Selection**.

3 Select Domain 2 only.

Create an explicit selection item for the well domain to be reused later.

4 Click **Create Selection**.

5 In the **Create Selection** dialog box, type `Well domain` 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	epsrW	1	Basic
Band gap	Eg0	EgW	V	Semiconductor material
Electron affinity	chi0	chiW	V	Semiconductor material
Effective density of states, valence band	Nv	Nv0	1/m³	Semiconductor material

Property	Variable	Value	Unit	Property group
Effective density of states, conduction band	Nc	Nc0	1/m³	Semiconductor material
Electron mobility	mun	mun0	m²/(V·s)	Semiconductor material
Hole mobility	mup	muLFW	m²/(V·s)	Semiconductor material

9 Right-click **Component 1 (comp1)>Materials>InSb Well** and choose **Duplicate**.

AlInSb Barrier

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **InSb Well 1 (mat2)**.

2 In the **Settings** window for **Material**, type `AlInSb Barrier` in the **Label** text field.

3 Select Domains 1, 3, 4, and 6 only.

Similarly create an explicit selection item for the barrier domains to be reused later.

4 Locate the **Geometric Entity Selection** section. Click **Create Selection**.

5 In the **Create Selection** dialog box, type `Barrier 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	epsrB	1	Basic
Band gap	Eg0	EgB	V	Semiconductor material
Electron affinity	chi0	chiB	V	Semiconductor material
Effective density of states, valence band	Nv	Nv0	1/m³	Semiconductor material
Effective density of states, conduction band	Nc	Nc0	1/m³	Semiconductor material

Property	Variable	Value	Unit	Property group
Electron mobility	mun	`mun0`	m²/(V·s)	Semiconductor material
Hole mobility	mup	`muLFB`	m²/(V·s)	Semiconductor material

Configure physics settings. Select the density-gradient formulation from the **Discretization** section of the main physics settings window. Specify the anisotropic density-gradient effective mass in the settings window for the **Semiconductor Material Model** domain feature. Note that even though the out-of-plane component is shown and editable, its value does not affect the result, since it appears as a common factor in the numerator and denominator of the inverse matrix formula, so it cancels out to give a common factor of 1 (except when it's zero, then zero divided by zero gives NaN, not 1). Therefore just leave its value as the default `me_const`.

SEMICONDUCTOR (SEMI)

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

2 Select Domains 1–4 and 6 only.

3 In the **Settings** window for **Semiconductor**, locate the **Domain Selection** section.

4 Click **Create Selection**.

5 In the **Create Selection** dialog box, type `Semiconductor domains` in the **Selection name** text field.

6 Click **OK**.

7 In the **Settings** window for **Semiconductor**, locate the **Thickness** section.

8 In the d text field, type `d0`.

9 Locate the **Model Properties** section. From the **Carrier statistics** list, choose **Fermi–Dirac**.

10 From the **Solution** list, choose **Majority carriers only**.

11 From the **Majority carriers** list, choose **Holes**.

12 Click to expand the **Discretization** section. From the **Formulation** list, choose **Finite element density-gradient (quadratic shape function)**.

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 `300[K]`.

4 Locate the **Material Properties, Density-Gradient** section. From the list, choose **Symmetric**.

5 In the $\mathbf{m}_h^{DG}$ table, enter the following settings:

mpDGpara	0	0
0	mpDGperp	0

For the hole mobility, select the **User defined** option and we will use variable definitions to implement the mobility model as specified by Eq. (3) in the reference paper. For the electric field component parallel to the local current density vector, even though it is a good enough approximation to just use the X component of the field (`semi.EX`), here we demonstrate how to instead use the built-in mobility model **Caughey-Thomas Mobility Model (E)** to obtain the parallel electric field component (`semi.smm1.mmct1.Epp`); an approach that is applicable to any general geometric arrangement.

6 Locate the **Mobility Model** section. From the μ_p list, choose **User defined**. In the associated text field, type `muptot`.

The variable is not yet defined, so it turns into yellow colored. Once it is defined, it will turn back to black colored. Now add the **Caughey-Thomas Mobility Model (E)** subnode. There is no need to enter any of the parameters, since the only purpose of this subnode is to provide the electric field component parallel to the local current density vector.

Caughey-Thomas Mobility Model (E) 1

In the **Physics** toolbar, click **Attributes** and choose **Caughey-Thomas Mobility Model (E)**.

Now define the mobility model variables; afterward the yellow variable should turn back to black colored. First define some physics setting parameters.

GLOBAL DEFINITIONS

Parameters 3: Physics

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters 3: Physics` in the **Label** text field.

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

Name	Expression	Value	Description
NaCap	5e20[cm^-3]	5E26 1/m³	p+ cap doping concentration
NaDelta	1e19[cm^-3]	1E25 1/m³	Delta doping concentration

Name	Expression	Value	Description
Vd	0[V]	0 V	Drain voltage
Vg	0[V]	0 V	Gate voltage

The low field mobility is different for different materials, as seen in the parameter definitions earlier. Create a common variable in each material domain(s) so that one single set of formulas for the mobility model can be shared among different materials. Use the explicit selection items defined earlier to streamline the process of selecting domains for the variable definition.

DEFINITIONS

Variables 1: Low field mobility, well

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 1: Low field mobility, well` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Well domain**.

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

Name	Expression	Unit	Description
mupLF	muLFW	$m^2/(V \cdot s)$	Low field mobility

6 Right-click **Variables 1: Low field mobility, well** and choose **Duplicate**.

Variables 2: Low field mobility, barrier

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Variables 1: Low field mobility, well 1**.

2 In the **Settings** window for **Variables**, type `Variables 2: Low field mobility, barrier` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Barrier domains**.

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

Name	Expression	Unit	Description
mupLF	muLFB	$m^2/(V \cdot s)$	Low field mobility

Variables 3: Mobility model

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Variables 3: Mobility model` in the **Label** text field.

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

Name	Expression	Unit	Description
`mupFDinv`	`sqrt(1+(mupLF*semi.smm1.mmct1.Epp/vSat)^2)/mupLF`	T	`Inverse of field dependent mobility`
`mupSSinv`	`(semi.EY/ESS)^4/muSS`	T	`Inverse of surface scattering mobility`
`muptot`	`1/(mupFDinv+mupSSinv)`	m²/(V·s)	`Total mobility`

Add doping features with continuation parameters to prepare for the ramp up of doping concentrations from small values in order to achieve better convergence.

SEMICONDUCTOR (SEMI)

Analytic Doping Model 1: p+ cap

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Analytic Doping Model 1: p+ cap` in the **Label** text field.

3 Select Domains 4 and 6 only.

4 Locate the **Impurity** section. In the N_{A0} text field, type `NaCap*cp`.

Analytic Doping Model 2: Delta doping

1 In the **Physics** toolbar, click **Domains** and choose **Analytic Doping Model**.

2 In the **Settings** window for **Analytic Doping Model**, type `Analytic Doping Model 2: Delta doping` in the **Label** text field.

3 Select Domain 3 only.

4 Locate the **Distribution** section. From the list, choose **Box**.

5 Locate the **Impurity** section. In the N_{A0} text field, type `NaDelta*cp`.

6 Locate the **Uniform Region** section. Specify the r_0 vector as

`-Ltot/2`	X
`-0.4*Htopbar`	Y

7 In the W text field, type `Ltot`.

8 In the D text field, type `0.2*Htopbar`.

9 Locate the **Profile** section. From the **Specify profile length scale** list, choose **Decay length**.

10 In the l_d text field, type `0.02*Htopbar`.

Add source, drain, and gate contacts. For the gate Schottky contact, zero out the effective Richardson constant for electrons to eliminate the possibility of unphysical electron current as a result of the majority carrier formulation for holes.

Metal Contact 1: Source

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

2 In the **Settings** window for **Metal Contact**, type `Metal Contact 1: Source` in the **Label** text field.

3 Select Boundary 9 only.

Metal Contact 2: Drain

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

2 In the **Settings** window for **Metal Contact**, type `Metal Contact 2: Drain` in the **Label** text field.

3 Select Boundary 19 only.

4 Locate the **Terminal** section. In the V_0 text field, type `Vd`.

Metal Contact 3: Gate

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

2 In the **Settings** window for **Metal Contact**, type `Metal Contact 3: Gate` in the **Label** text field.

3 Select Boundary 13 only.

4 Locate the **Terminal** section. In the V_0 text field, type `Vg`.

5 Locate the **Contact Type** section. From the **Type** list, choose **Ideal Schottky**.

6 Locate the **Contact Properties** section. From the **Barrier height** list, choose **User defined**. In the Φ_B text field, type `PhiB`.

7 Locate the **Thermionic Currents** section. In the A^*_n text field, type `0[A/(K*cm)^2]`.

Add quantum confinement effect at the top barrier layer boundaries (the top barrier-vacuum interfaces). Use a large value for the barrier height to simulate the infinite barrier for holes.

Insulation 2

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

2 Select Boundaries 11 and 16 only.

3 In the **Settings** window for **Insulation**, locate the **Density-Gradient** section.

4 From the **Formulation** list, choose **Potential barrier**.

5 In the Φ_p^{Ox} text field, type `1000[V]`.

Use the **Distribution** feature to help create an efficient **Mapped** mesh that minimizes the number of mesh elements while still resolving large gradients in the solution fields.

MESH 1

Edge 1

1 In the **Mesh** toolbar, click **More Generators** and choose **Edge**.

2 Select Boundaries 11 and 16 only.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `20`.

5 In the **Element ratio** text field, type `5`.

6 Select the **Symmetric distribution** check box.

Edge 1

In the **Model Builder** window, right-click **Edge 1** and choose **Duplicate**.

Edge 2

1 In the **Model Builder** window, click **Edge 2**.

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

3 Click **Clear Selection**.

4 Select Boundary 13 only.

Distribution 1

1 In the **Model Builder** window, expand the **Edge 2** node, then click **Distribution 1**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 In the **Number of elements** text field, type `10`.

4 In the **Element ratio** text field, type `2.5`.

Edge 2

In the **Model Builder** window, right-click **Edge 2** and choose **Duplicate**.

Edge 3

1. In the **Model Builder** window, click **Edge 3**.
2. In the **Settings** window for **Edge**, locate the **Boundary Selection** section.
3. Click  **Clear Selection**.
4. Select Boundary 8 only.

Distribution 1

1. In the **Model Builder** window, expand the **Edge 3** node, then click **Distribution 1**.
2. In the **Settings** window for **Distribution**, locate the **Distribution** section.
3. In the **Number of elements** text field, type `12`.
4. In the **Element ratio** text field, type `6`.
5. Clear the **Symmetric distribution** check box.

Edge 3

In the **Model Builder** window, right-click **Edge 3** and choose **Duplicate**.

Edge 4

1. In the **Model Builder** window, click **Edge 4**.
2. In the **Settings** window for **Edge**, locate the **Boundary Selection** section.
3. Click  **Clear Selection**.
4. Select Boundary 18 only.

Copy Edge 1

1. In the **Model Builder** window, right-click **Mesh 1** and choose **Copying Operations> Copy Edge**.
2. Select Boundaries 8, 11, 13, 16, and 18 only.
3. In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.
4. Click to select the  **Activate Selection** toggle button.
5. Select Boundaries 2, 4, and 6 only.

Copy Edge 2

1. Right-click **Mesh 1** and choose **Copying Operations>Copy Edge**.
2. Select Boundaries 8 and 18 only.
3. In the **Settings** window for **Copy Edge**, locate the **Destination Boundaries** section.

4 Click to select the **Activate Selection** toggle button.

5 Select Boundaries 9 and 19 only.

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 From the **Selection** list, choose **Semiconductor domains**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 22 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 20.

6 In the **Element ratio** text field, type 5.

7 Select the **Symmetric distribution** check box.

8 Right-click **Distribution 1** and choose **Duplicate**.

Distribution 2

1 In the **Model Builder** window, click **Distribution 2**.

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

3 Click **Clear Selection**.

4 Select Boundaries 3 and 21 only.

5 Locate the **Distribution** section. In the **Number of elements** text field, type 10.

6 Right-click **Distribution 2** and choose **Duplicate**.

Distribution 3

1 In the **Model Builder** window, click **Distribution 3**.

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

3 Click **Clear Selection**.

4 Select Boundaries 7, 10, 17, and 23 only.

5 Locate the **Distribution** section. In the **Element ratio** text field, type 10.

6 Clear the **Symmetric distribution** check box.

7 Right-click **Distribution 3** and choose **Duplicate**.

Distribution 4

1 In the **Model Builder** window, click **Distribution 4**.

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

3 Click **Clear Selection**.

4 Select Boundaries 1 and 20 only.

5 Locate the **Distribution** section. In the **Number of elements** text field, type `25`.

6 In the **Element ratio** text field, type `50`.

7 Select the **Reverse direction** check box.

8 Click **Build All**.

Use the **Auxiliary sweep** feature to ramp up the doping concentrations and band offsets from small values in order to achieve better convergence. The built-in mobility model **Caughey-Thomas Mobility Model (E)** creates additional degrees of freedom to solve the implicit equations for the parallel electric field components. At this stage it is not necessary to solve those equations, since here we only solve for the equilibrium state to provide a good initial condition for subsequent studies. Therefore disable the mobility model node in the **Modify model configuration for study step** window.

STUDY 1: RAMP DOPING AND BAND OFFSET

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

2 In the **Settings** window for **Study**, type `Study 1: Ramp doping and band offset` in the **Label** text field.

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

Step 1: Semiconductor Equilibrium

1 In the **Model Builder** window, under **Study 1: Ramp doping and band offset** click **Step 1: Semiconductor Equilibrium**.

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

3 Select the **Modify model configuration for study step** check box.

4 In the tree, select **Component 1 (comp1)>Semiconductor (semi)> Semiconductor Material Model 1>Caughey-Thomas Mobility Model (E) 1**.

5 Click **Disable**.

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

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
cp (Continuation parameter for heterojunction and doping)	`10^range(-12,4,0)`	

9 In the table, click to select the cell at row number 1 and column number 3.

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

Add a study to sweep the drain and gate voltages, using the solution from the previous study as the initial condition. The voltages are swept from 0 (equilibrium) up to the starting point of the next study. The result of this study will be used as the initial condition for the next study, which will do a further sweep to produce the I-V curve. Set "reuse solution" to "Yes".

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

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary

1 In the **Settings** window for **Stationary**, click to expand the **Values of Dependent Variables** section.

2 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

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

4 From the **Study** list, choose **Study 1: Ramp doping and band offset, Semiconductor Equilibrium**.

5 From the **Parameter value (cp)** list, choose **Last**.

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

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vd (Drain voltage)	`0 -0.1 -0.3 -0.5`	V

9 In the table, click to select the cell at row number 1 and column number 3.

10 Click + **Add**.

11 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`0 -0.1 -0.4 -0.6`	V

12 In the table, click to select the cell at row number 2 and column number 3.

13 From the **Reuse solution from previous step** list, choose **Yes**.

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

15 In the **Settings** window for **Study**, type `Study 2: Ramp Vd and Vg (only as init cond for next study)` 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**.

Add a study to sweep the gate voltage for the Id-Vg curve, using the solution from the previous study as the initial condition.

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

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3: VG SWEEP FOR ID-VG CURVE

1 In the **Settings** window for **Stationary**, locate the **Values of Dependent Variables** section.

2 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

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

4 From the **Study** list, choose **Study 2: Ramp Vd and Vg (only as init cond for next study), Stationary**.

5 From the **Parameter value (Vg (V),Vd (V))** list, choose **Last**.

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

7 From the **Sweep type** list, choose **All combinations**.

8 Click + **Add**.

9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vd (Drain voltage)	`-0.5`	V

10 In the table, click to select the cell at row number 1 and column number 3.

11 Click + **Add**.

12 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Vg (Gate voltage)	`range(-0.6,0.1,0.6)`	V

13 In the table, click to select the cell at row number 2 and column number 3.

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

15 In the **Settings** window for **Study**, type `Study 3: Vg sweep for Id-Vg curve` in the **Label** text field.

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

RESULTS

N-type

The model has only p-type dopant therefore, the n-type part of the default generated plot is not needed.

1 In the **Model Builder** window, expand the **Net Dopant Concentration (semi)** node.

2 Right-click **N-type** and choose **Delete**.

Plot the Id-Vg curve to be compared with Fig. 8 in the reference paper.

Id-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-Vg` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Vg sweep for Id-Vg curve/ Solution 3 (sol3)**.

4 Locate the **Axis** section. Select the **Manual axis limits** check box.

5 In the **x minimum** text field, type `-0.7`.

6 In the **x maximum** text field, type `0.6`.

7 In the **y minimum** text field, type `0.1`.

8 In the **y maximum** text field, type `500`.

9 Select the **y-axis log scale** check box.

Global 1

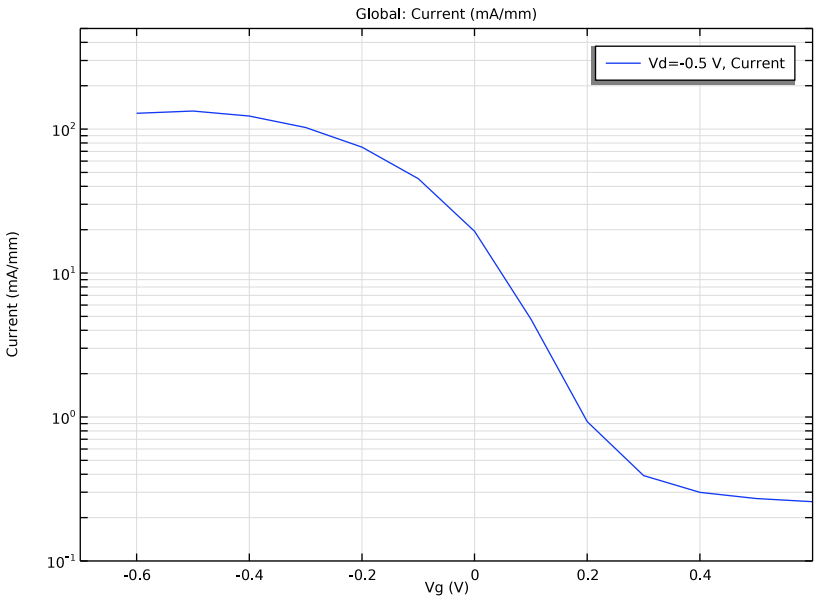
1 Right-click **Id-Vg** and choose **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`-semi.IO_2/dO`	`mA/mm`	`Current`

4 In the **Id-Vg** toolbar, click **Plot**.



Adjust the hole concentration plot to be compared with Fig. 7 in the reference paper. Optionally, if interested, use a Grid dataset to add some lines to represent the gate domain which is not explicitly modeled.

Hole Concentration (semi)

1 In the **Model Builder** window, under **Results** click **Hole Concentration (semi)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Parameter value (Vg (V))** list, choose **0.3**.

Surface 1

1 In the **Model Builder** window, expand the **Hole Concentration (semi)** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click to expand the **Range** section.

3 Select the **Manual color range** check box.

4 In the **Minimum** text field, type `10^10`.

5 In the **Maximum** text field, type `10^21`.

Grid 1D 1: Only for adding lines in 2D plot

1 In the **Results** toolbar, click **More Datasets** and choose **Grid>Grid 1D**.

2 In the **Settings** window for **Grid 1D**, type `Grid 1D 1: Only for adding lines in 2D plot` in the **Label** text field.

3 Locate the **Parameter Bounds** section. In the **Name** text field, type `s`.

4 In the **Maximum** text field, type `1e9`.

Line 1

1 In the **Model Builder** window, right-click **Hole Concentration (semi)** and choose **Line**.

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

3 From the **Dataset** list, choose **Grid 1D 1: Only for adding lines in 2D plot**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

5 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

6 From the **Color** list, choose **Black**.

Deformation 1

1 Right-click **Line 1** and choose **Deformation**.

2 In the **Settings** window for **Deformation**, locate the **Expression** section.

3 In the **x-component** text field, type `-root.s-Lgate/2`.

4 In the **y-component** text field, type `root.s*Hcap`.

5 Locate the **Scale** section.

6 Select the **Scale factor** check box. In the associated text field, type `1`.

Line 1

In the **Model Builder** window, right-click **Line 1** and choose **Duplicate**.

Deformation 1

1 In the **Model Builder** window, expand the **Line 2** node, then click **Deformation 1**.

2 In the **Settings** window for **Deformation**, locate the **Expression** section.

3 In the **x-component** text field, type `-root.s+Lgate/2`.

Line 2

In the **Model Builder** window, right-click **Line 2** and choose **Duplicate**.

Deformation 1

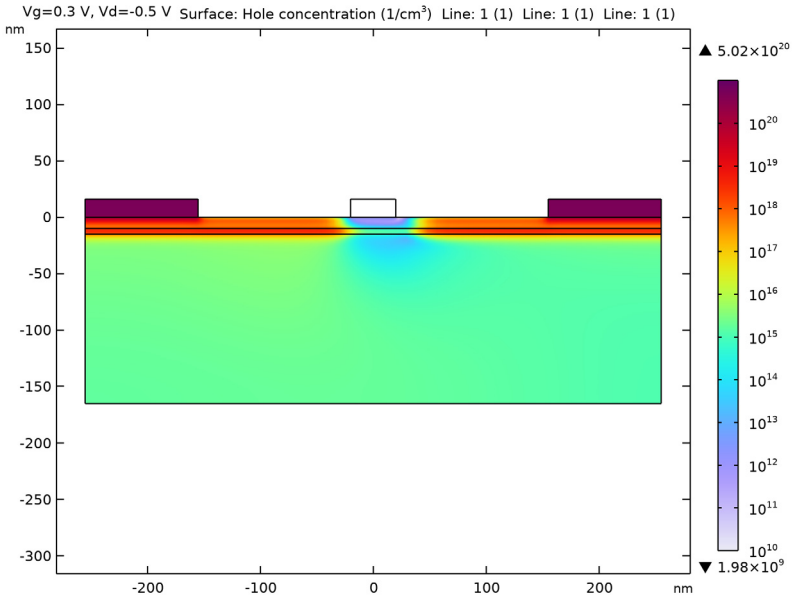
1 In the **Model Builder** window, expand the **Line 3** node, then click **Deformation 1**.

2 In the **Settings** window for **Deformation**, locate the **Expression** section.

3 In the **x-component** text field, type `-root.s-Lgate/2+root.s*Lgate`.

4 In the **y-component** text field, type `Hcap`.

5 In the **Hole Concentration (semi)** toolbar, click **Plot**.



As an example to show the quantum confinement effects introduced by the density-gradient formulation, compare the hole density profile with an approximate drift-diffusion profile on a cut line. The model is not recomputed, instead, to save time, the valence band

edge and the quasi-Fermi level for the holes (both also plotted) are used in the drift-diffusion formula as is, to provide a crude approximation for the qualitative comparison. The effect of confinement in both the quantum well and the top barrier-vacuum interface (y = 0 nm) is clearly seen in the difference in the shapes of the profiles of the hole concentration.

Cut Line 2D 1

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

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

3 From the **Dataset** list, choose **Study 3: Vg sweep for Id-Vg curve/Solution 3 (sol3)**.

4 Locate the **Line Data** section. In row **Point 1**, set **X** to `-100[nm]`.

5 In row **Point 2**, set **X** to `-100[nm]`.

6 In row **Point 2**, set **Y** to `-30[nm]`.

Hole Concentration Line Cut

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

2 In the **Settings** window for **1D Plot Group**, type `Hole Concentration Line Cut` in the **Label** text field.

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

4 From the **Parameter selection (Vg)** list, choose **From list**.

5 In the **Parameter values (Vg (V))** list, select **0.3**.

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

7 In the **Title** text area, type `Hole concentration:density-gradient(DG) vs. drift-diffusion(DD), Valence band edge(Ev), Hole quasi-Fermi level(Efp)`.

8 Locate the **Plot Settings** section. Select the **Two y-axes** check box.

9 Select the **Secondary y-axis label** check box. In the associated text field, type `Energy levels (eV)`.

10 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

Line Graph 1

1 Right-click **Hole Concentration Line Cut** and choose **Line Graph**.

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

3 In the **Expression** text field, type `semi.P`.

4 In the **Unit** field, type `1/cm^3`.

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

6 In the **Expression** text field, type `y`.

7 Click to expand the **Legends** section. Select the **Show legends** check box.

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
P (DG)

10 Right-click **Line Graph 1** and choose **Duplicate**.

Line Graph 2

1 In the **Model Builder** window, click **Line Graph 2**.

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

3 In the **Expression** text field, type `semi.Nv*semi.FD_half((semi.Ev-semi.Efp)/semi.Vth)`.

4 Select the **Description** check box. In the associated text field, type `Hole concentration`.

5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

6 From the **Color** list, choose **Red**.

7 Locate the **Legends** section. In the table, enter the following settings:

Legends
P (DD)

8 Right-click **Line Graph 2** and choose **Duplicate**.

Line Graph 3

1 In the **Model Builder** window, click **Line Graph 3**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis** section.

3 Select the **Plot on secondary y-axis** check box.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `semi.Ev`.

5 Locate the **Legends** section. In the table, enter the following settings:

Legends
Ev

6 Locate the **y-Axis Data** section. Clear the **Description** check box.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

8 From the **Color** list, choose **Cycle**.

9 Right-click **Line Graph 3** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

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

3 In the **Expression** text field, type `semi.Efp`.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 From the **Color** list, choose **Black**.

6 Locate the **Legends** section. In the table, enter the following settings:

Legends
Efp

7 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

8 In the **Hole Concentration Line Cut** toolbar, click **Plot**.