INTRODUCTION TO

Semiconductor Module

COMSOL

Introduction to the Semiconductor Module

Version: COMSOL 6.3

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Introduction

Device engineers and physicists use the Semiconductor Module to design and optimize semiconductor devices. For many years semiconductor device design has been closely associated with the use of simulation tools, due to the high cost of prototyping new devices and processes. The advance of nanotechnology and organic semiconductors has helped create many novel devices. Researchers in these fields also use simulation to assist the fundamental understanding and design optimization. For all of the systems mentioned above, multiphysics effects often play an important role, and COMSOL Multiphysics is the ideal platform for investigating these effects.

The Semiconductor Module includes a predefined Semiconductor interface, which is based on the conventional *drift–diffusion* formulation. An optional *density-gradient* implementation is also available to provide a computationally efficient method to add the effect of quantum confinement to the drift–diffusion equation system.

In addition, a predefined Schrödinger Equation interface and a predefined Schrödinger–Poisson Equation multiphysics interface allow more detailed modeling of quantum-confined systems such as quantum wells, wires, and dots.

The Semiconductor Module enables the stationary and dynamic performance of devices to be modeled in one, two, and three dimensions, together with circuit-based modeling of active and passive devices. In the frequency domain, it is possible to model devices driven by a combination of AC and DC signals. A broad range of semiconductor devices can be modeled, and phenomena such as heat generation, electrochemical reaction, and optoelectronic effects can be straightforwardly included using predefined or manual couplings.

The Semiconductor interface solves the drift–diffusion and Poisson's equations by either the finite volume or the finite element method. The physics interface solves a set of coupled partial differential equations for the electric potential and for the electron and hole concentrations (or their logarithm in the case of the finite element method log formulation, or their quasi-Fermi levels in the case of the quasi-Fermi level and density-gradient formulation). The corresponding initial and boundary conditions are easily specified in the physics interface.

The COMSOL Multiphysics design emphasizes the physics by providing users with the equations solved by each feature and by offering full access to the underlying equation system. The *Semiconductor Module User's Guide* provides complete information on the theory underlying the Semiconductor interface.

There is also tremendous flexibility to add user-defined equations and expressions to the system. For example, user-defined mobility models can be readily specified simply by typing appropriate expressions into the user defined feature, no scripting

or coding is required. These user-defined mobility models can be combined arbitrarily with the predefined mobility models built into the software. When COMSOL Multiphysics compiles the equations, the complex couplings generated by these user-defined expressions are automatically included in the equation system. The equations are then solved using a range of state-of-the-art solvers.

Once a solution is obtained, a large range of result analysis tools are available to interrogate the data, and predefined plots are automatically generated to show the device response. COMSOL Multiphysics offers the flexibility to evaluate a wide range of physical quantities including predefined quantities such as the electron and hole currents (including current components from drift, diffusion, and thermal diffusion), the electric field, the generation–recombination rate, and the temperature, all available through easy-to-use menus, as well as arbitrary user-defined expressions.

To model a Semiconductor device, the geometry is first defined in the software. Then appropriate materials are selected and the Semiconductor interface is added. The dopant distribution can be computed separately using a diffusion equation calculation, imported from third party software, or specified empirically using the built-in doping features. Initial conditions and boundary conditions are set up within the physics interface. Next, the mesh is defined and a solver is selected. Finally the results are visualized using a wide range of plotting and evaluation tools. All of these steps are accessed from the intuitive COMSOL Desktop graphical user interface.

The Schrödinger Equation interface solves the Schrödinger equation for the wave function of a single particle in an external potential. This can be applied to general quantum mechanical problems, as well as for the electron and hole wave functions in quantum-confined systems under the envelope function approximation. Appropriate boundary conditions and study types are implemented for the user to easily set up models to compute relevant quantities in various situations, such as the eigenenergies of bound states, the decay rates of quasi bound states, the transmission and reflection coefficients, the resonant tunneling condition, and the effective band gap of a superlattice structure. The Double Barrier 1D, Superlattice Band Gap Tool, and k dot p Method for Strained Wurtzite GaN Band Structure models in the Application Libraries illustrate the usage of the various built-in functionalities.

Semiconductor Devices

The Semiconductor Module can be applied to solve a range of device simulation problems. The Semiconductor interface can be straightforwardly coupled with other physics interfaces, such as the Electromagnetic waves interfaces (using the predefined Semiconductor Optoelectronics multiphysics coupling), the Heat Transfer in Solids interface and the Electrical Circuits interface. Coupling to a circuit is straightforward using the terminals included with appropriate boundary conditions. Figure 1 shows results obtained from a 2D p–n junction model in which a device model of a diode is coupled to an electrical circuit to produce a rectifier. The electron and hole concentrations are shown in the plots when different voltages are applied to the circuit.
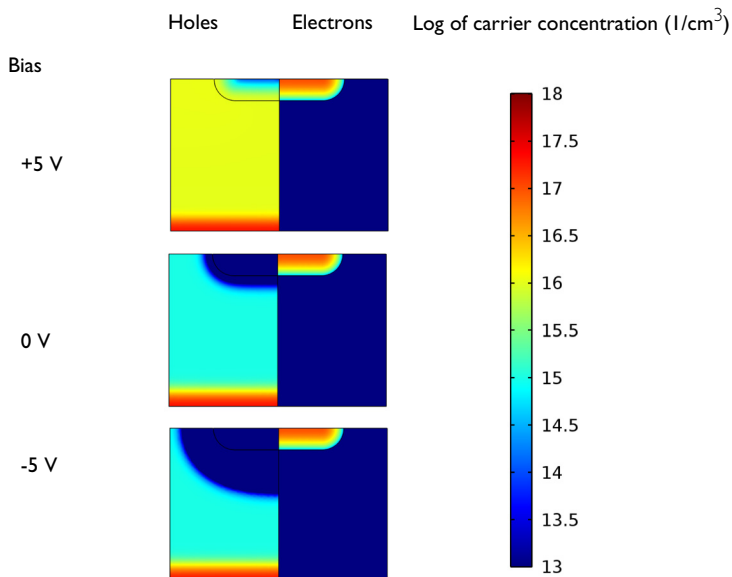
Figure 1: Electron and hole concentrations in a p–n junction diode connected to a series resistor under different bias conditions. This plot shows clearly the changing geometry and extent of the depletion region under reverse bias.

A range of common device types can be simulated with the module, including MOSFETs, MESFETs, JFETs, diodes, and bipolar transistors. These devices can be analyzed for the steady state, in the time domain or in the frequency

domain (with mixed DC and AC signals, using the small signal analysis study type).

A number of standard analyses are illustrated with the MOSFET model series, which shows how to include a range of increasingly complicated semiconductor physics effects using features included within the Semiconductor interface. The first model in the MOSFET series is described in the section Tutorial Model: DC Characteristics of a MOSFET, below. Figure 2 shows some of the results obtained from this analysis.
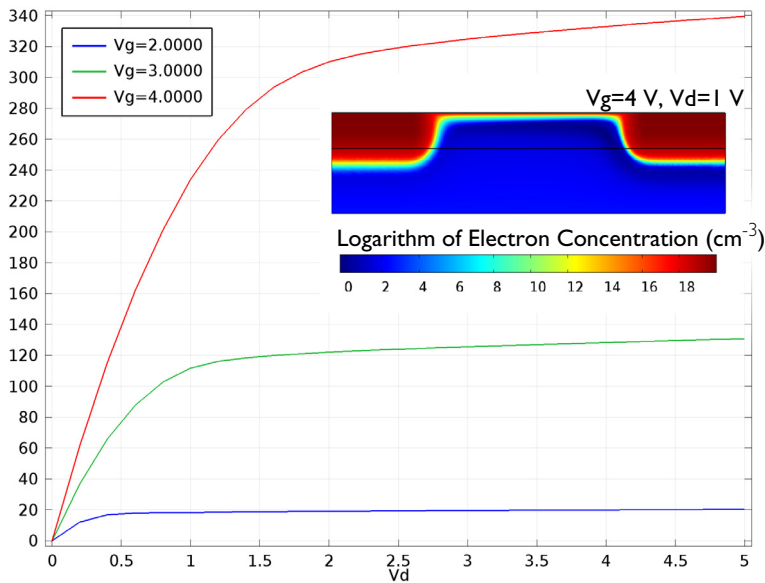

Figure 2: Stationary analysis of a MOSFET. The plot shows the drain current plotted against the drain voltage (V_d) for a range of different values of the gate voltage (V_g) The inset shows the logarithm of the electron concentration (in units of cm^{-3}) for a gate voltage of 4 V and for a drain voltage of 1 V. The channel is clearly visible.

In addition to the MOSFET model series, a wide array of other example models are available. The Bipolar Transistor model sequence gives an example of how to set up a multiphysics device simulation. Initially, a model of a 2D cross section of a bipolar transistor device is created using only the Semiconductor interface. This model is then extended by two other models in the sequence, one adds coupling to the Heat Transfer interface and the other demonstrates how to create a full 3D simulation of the same device.

The MOSCAP model series shows different ways of analyzing this fundamental building block of many devices. The ISFET model demonstrates the coupling to

the electrochemistry physics. The Heterojunction Tunneling model shows how to add tunneling current contributions using the WKB approximation. The Interface Trapping Effects of A MOSCAP model does what its name suggests. The pair of models Reverse Recovery of a PIN Diode and Forward Recovery of a PIN Diode demonstrates the modeling of carrier dynamics with a time dependent study.

Several individual models are also provided, including a MESFET, an EEPROM device, a solar cell, a photodiode, and some LED models. Figure 3 shows the electron and hole currents flowing in a simple 2D Bipolar transistor.
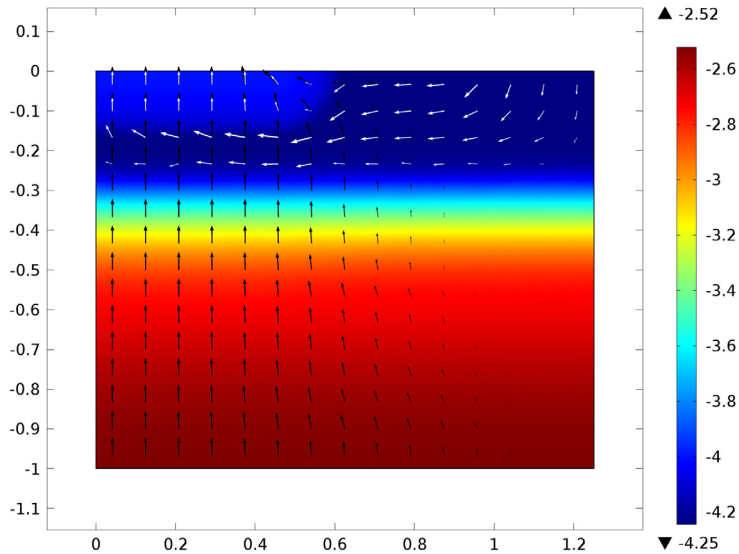
Figure 3: Electric potential in V (color) and direction of the current flow for electrons (black arrows) and holes (white arrows) in a simple 2D bipolar transistor.

The density-gradient formulation is demonstrated in a 1D inversion layer, a 2D FET, and a 3D nanowire model. The last one is shown in Figure 4.
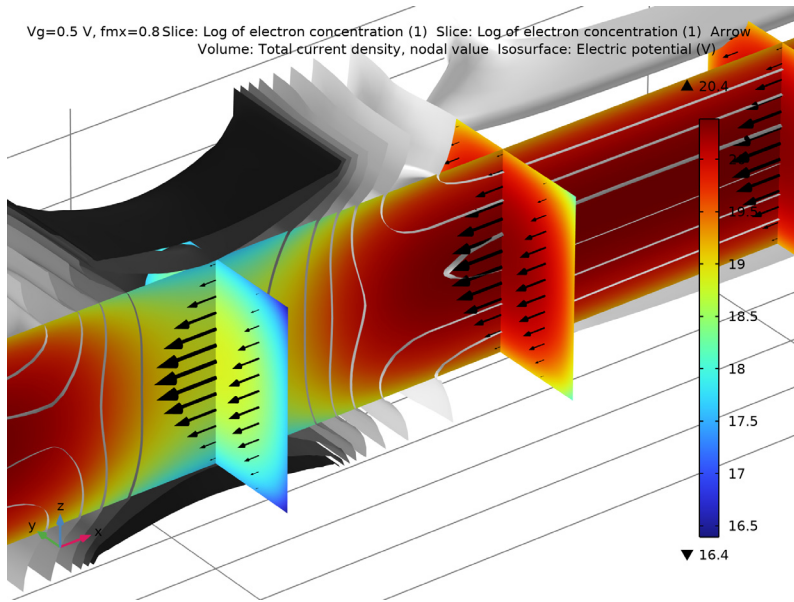
Figure 4: Electron concentration (color), electric potential (isosurface), and total current density (arrow) of a 3D nanowire model with the quantum confinement effect included using the density-gradient formulation.

The Schrödinger Equation interface enables the modeling of various quantum-confined systems. The following graph shows the wave functions shifted by the respective energy levels for the resonant tunneling conditions of a double barrier structure.
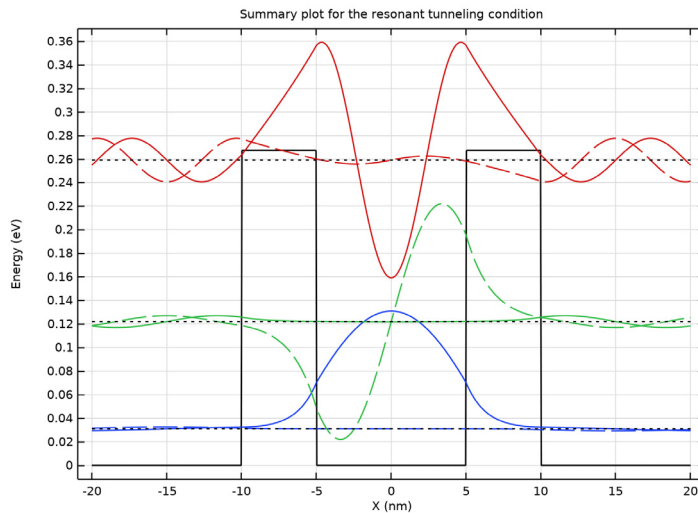
The Schrödinger–Poisson Equation interface adds the Electrostatics physics to take into account the effects of the charge density of the carriers. The following graph shows the self-consistent result of electrons confined in a quantum wire.
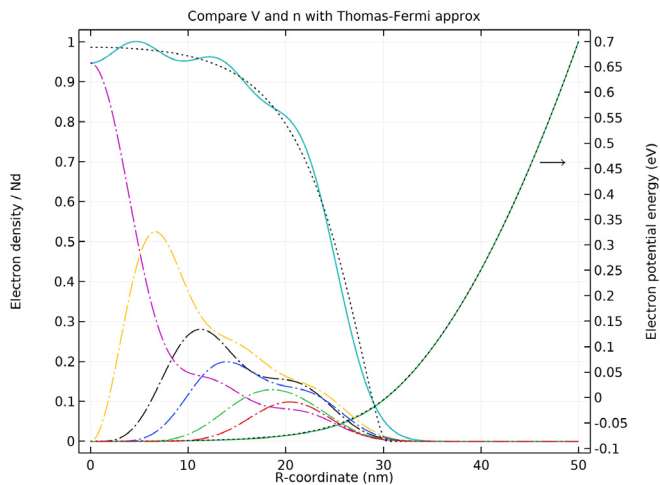
Each COMSOL Multiphysics physics interface (for example, the Semiconductor interface or the Schrödinger Equation interface) expresses the relevant physical phenomena in the form of sets of partial or ordinary differential equations, together with appropriate boundary and initial conditions. Each feature added to the physics interface represents a term or condition in the underlying equation set. These features are usually associated with a geometric entity within the model, such as a domain, boundary, edge, or point.

Figure 5 uses a model similar to the MOSFET application library example to show the Model Builder tree structure, and the Settings window for the selected Semiconductor Material Model 1 feature node. This node adds the semiconductor equations to the simulation within the domains selected. In the Model Inputs section the temperature of the material is specified. It is straightforward to link this temperature to a separate Heat Transfer interface to solve nonisothermal problems — the Semiconductor interface automatically defines an appropriate heat source term that can be readily accessed in a Heat Transfer interface. In the Material Properties section, the Settings window indicates that the relative permittivity and the band gap are inherited from the material properties assigned to the domain. The material properties can be set up as functions of other dependent variables in the model, for example, the temperature. The dopant density is specified by means of multiple additive doping features, which can be used to combine Gaussian and user-defined dopant density profiles to produce the desired profile. Several boundary conditions are also indicated in the model tree. The Ohmic Contact boundary condition is commonly used to model nonrectifying interconnects. The Thin Insulating Gate feature models a gate with a thickness smaller than the typical length scale of the mesh. It is also possible to model gates explicitly, solving Poisson's equation within the dielectric.

Model Builder

- Untitled.mph *(root)*
  - Global Definitions
    - Parameters 1
    - Default Model Inputs
    - Materials
  - Component 1 *(comp 1)*
    - Definitions
    - Geometry 1
    - Materials
    - Semiconductor *(semi)*
      - Semiconductor Material Model 1
      - Insulation 1
      - Zero Charge 1
      - Insulator Interface 1
      - Continuity/Heterojunction 1
      - Initial Values 1
      - Analytic Doping Model 1
      - Analytic Doping Model 2
      - Geometric Doping Model 1
      - Metal Contact 1
      - Metal Contact 2
      - Thin Insulator Gate 1
      - Trap-Assisted Surface Recombination 1
      - Trap-Assisted Recombination 1
    - Mesh 1
  - Study 1
  - Results

Highlighted node shown in settings window → Semiconductor Material Model 1

Additive doping features → Analytic Doping Model 1, Analytic Doping Model 2

Boundary conditions → Metal Contact 1

Equations added by the feature

Material temperature

Material properties are obtained from the built-in material library in this model

Settings

Semiconductor Material Model

Label: Semiconductor Material Model 1

▼ Domain Selection

Selection: All domains

1

▷ Override and Contribution

▼ Equation

Show equation assuming:

Study 1, Stationary

$\rho + = q(p - n + N_d^+ - N_a^-)$

$\nabla \cdot \mathbf{J}_n = 0, \quad \nabla \cdot \mathbf{J}_p = 0$

$\mathbf{J}_n = qn\mu_n \nabla E_c + qD_n \nabla n - qnD_n \nabla \ln(N_c) + qnD_{n,th} \nabla \ln(T)$

$\mathbf{J}_p = qp\mu_p \nabla E_v - qD_p \nabla p + qpD_p \nabla \ln(N_v) - qpD_{p,th} \nabla \ln(T)$

$E_c = -(V + \chi_0), \quad E_v = -(V + \chi_0 + E_{g,0})$

▼ Model Input

Temperature:

T User defined

293.15[K] K

▼ Material Properties

Relative permittivity:

ϵ_r From material

Band gap:

$E_{g,0}$ From material

Electron affinity:

χ_0 From material

Effective density of states, valence band:

N_v From material

Effective density of states, conduction band:

N_c From material

Figure 5: The Model Builder (to the left), and the Settings window for Semiconductor Material Model1 for the selected feature node (to the right). The Equation section in the Settings window shows the model equations.

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The Semiconductor interface is the starting point for most simulations. The Semiconductor Module also includes physics interfaces to enable modeling of different physical situations encountered in device design. When a new model is started, these physics interfaces are selected from the Model Wizard.

Figure 6 shows the physics interfaces included with the Semiconductor Module. The two Semiconductor Optoelectronics interfaces are only available with an additional Wave Optics module license.
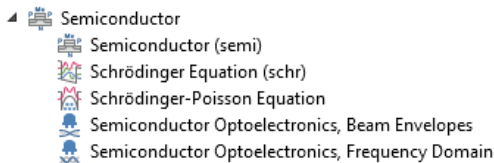

Figure 6: The Semiconductor Module interfaces as displayed in the Model Wizard for a 3D model. The Semiconductor Optoelectronics interfaces are only available with an additional Wave Optics Module license.

Also see Physics Interface Guide by Space Dimension and Study Type. Below, a brief overview of each of the Semiconductor Module physics interfaces is given.

ELECTROSTATICS

The Electrostatics interface ( ), found under the AC/DC branch in the Model Wizard, solves for the electric potential given the charge distribution in the domain and the voltages applied to boundaries. It is used to model electrostatic devices under static or quasistatic conditions, that is at frequencies sufficiently low that wave propagation effects can be neglected. Many of the features of the Electrostatics interface are included in the Semiconductor interface, where they affect the solution of the electric potential.

ELECTRICAL CIRCUIT

The Electrical Circuit interface ( ), found under the AC/DC branch in the Model Wizard, has the equations to model electrical circuits with or without connections to a distributed fields model. The interface solves for the voltages, currents, and charges associated with the circuit elements. Circuit models can contain passive elements like resistors, capacitors, and inductors as well as active elements such as diodes and transistors. Circuits can be imported from an existing SPICE net list. A typical application of this interface would be to consider the effect of series or parallel lumped components on device behavior.

TRANSPORT OF CHARGE CARRIERS

The Transport of Charge Carriers interface ( ) is used to solve the number density of one or multiple charge carriers. The charge carriers can be charged species such as electrons, ions, and neutral species like molecules and their excited states. Transport and reactions of charge carriers can be handled with this interface. The driving forces for transport can be drift when coupled to an electromagnetic field, convection when coupled to a flow field, and diffusion.

SEMICONDUCTOR

The Semiconductor interface ( ), found under the Semiconductor branch in the Model Wizard, solves the drift–diffusion and Poisson's equations. The physics interface allows both insulating and semiconducting domains to be modeled. The equations account fully for thermal effects, and the interface can be coupled to a heat transfer interface using the temperature model input and the predefined heat source term. This physics interface is appropriate for modeling semiconductor devices.

SEMICONDUCTOR OPTOELECTRONICS, BEAM ENVELOPES

The Semiconductor Optoelectronics, Beam Envelopes ( ) multiphysics interface combines the Semiconductor interface with the Electromagnetic Waves, Beam Envelopes interface. The coupling occurs through the Optical Transitions feature, which adds a stimulated emission generation term (appropriate for direct band-gap materials) on domains in the Semiconductor interface. This term is proportional to the optical intensity in the corresponding Wave Equation, Beam Envelopes feature in the Electromagnetic Waves, Beam Envelopes interface. Additionally spontaneous emission (for direct band-gap materials) can be accounted for. The effect of the light adsorption or emission is accounted for by a corresponding change in the complex permittivity or refractive index in the Wave Equation, Beam Envelopes feature.

This multiphysics interface can be used for modeling devices such as photodiodes, light emitting diodes and laser diodes without quantum wells in direct band gap materials.

SEMICONDUCTOR OPTOELECTRONICS, FREQUENCY DOMAIN

The Semiconductor Optoelectronics, Frequency Domain ( ) multiphysics interface combines the Semiconductor interface with the Electromagnetic Waves, Frequency Domain interface. The coupling occurs through the Optical Transitions feature, which adds a stimulated emission generation term (appropriate for direct band-gap materials) on domains in the Semiconductor interface. This term is proportional to the optical intensity in the corresponding

Wave Equation, Electric feature in the Electromagnetic Waves, Frequency Domain interface. Additionally spontaneous emission (for direct band-gap materials) is accounted for. The effect of the light adsorption or emission is accounted for by a corresponding change in the complex permittivity or refractive index in the Wave Equation, Electric feature.

This multiphysics interface can be used for modeling devices such as photodiodes, light emitting diodes and laser diodes without quantum wells in direct band gap materials.

SCHRÖDINGER EQUATION

The Schrödinger Equation interface ( ), found under the Semiconductor branch in the Model Wizard, solves the Schrödinger equation for a single particle in an external potential. This physics interface is useful for general quantum mechanical problems as well as for quantum confined systems such as quantum wells, wires, and dots (with the envelope function approximation).

SCHRÖDINGER–POISSON EQUATION

The Schrödinger–Poisson Equation multiphysics interface ( ) combines the Schrödinger Equation interface with the Electrostatics interface to model charge carriers in quantum-confined systems. The electric potential from the Electrostatics contributes to the potential energy term in the Schrödinger Equation. A statistically weighted sum of the probability densities from the eigenstates of the Schrödinger Equation contributes to the space charge density in the Electrostatics. A dedicated Schrödinger–Poisson Study Type is available to automatically generate the solver sequence iterations for the self-consistent solution of the bidirectionally coupled system.

This multiphysics interface can be used for modeling quantum confined devices such as quantum wells, wires, and dots.

Physics Interface Guide by Space Dimension and Study Type

The table below lists the physics interfaces available specifically with this module in addition to the COMSOL Multiphysics basic license.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
⚡ **AC/DC**				
Electrical Circuit		cir	Not space dependent	stationary; frequency domain; time dependent; frequency domain; eigenfrequency
Electrostatics[1]		es	all dimensions	stationary; time dependent; stationary source sweep; eigenfrequency; frequency domain; small signal analysis, frequency domain
Electric Discharge				
Transport of Charge Carriers		tcc	all dimensions	time dependent; stationary; frequency domain perturbation
Semiconductor				
Semiconductor		semi	all dimensions	small-signal analysis, frequency domain; stationary; time dependent; semiconductor equilibrium
Semiconductor Optoelectronics, Beam Envelopes[2]		—	3D, 2D, and 2D axisymmetric	frequency-stationary; frequency-transient; small-signal analysis, frequency domain
Semiconductor Optoelectronics, Frequency Domain[2]		—	3D, 2D, and 2D axisymmetric	frequency-stationary; frequency-transient; small-signal analysis, frequency domain
Schrödinger Equation		schr	all dimensions	eigenvalue; stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Schrödinger-Poisson Equation		—	all dimensions	Schrödinger-Poisson

[1] This physics interface is included with the core COMSOL package but has added functionality for this module.

[2] Requires both the Wave Optics Module and the Semiconductor Module.

Learning Resources

In addition to the tutorial model in the next section (Tutorial Model: DC Characteristics of a MOSFET), there are many examples in the Application Libraries. Every example is accompanied by a PDF documentation with step-by-step instructions and useful comments. The examples can be accessed either online (https://www.comsol.com/models/semiconductor-module) or within the software by going to the File menu > Application Libraries > Semiconductor Module.

For users interested in the drift–diffusion type of formulations, we recommend to start with the simple model of a p–n junction with user-defined generation for a silicon solar cell: https://www.comsol.com/model/si-solar-cell-1d-35661. This gives a quick introduction to building a semiconductor model from scratch.

Next, the 1D heterojunction model demonstrates standard techniques to achieve convergence (see comments in the accompanying PDF documentation): https://www.comsol.com/model/heterojunction-1d-14617.

The tutorial in the next section shows a simple 2D model. More 2D models can be found in the Application Libraries.

To model the oxide domain explicitly, use the Charge Conservation domain condition, as shown in this example of an EEPROM: https://www.comsol.com/model/programming-of-a-floating-gate-eeprom-device-18075.

For users interested in the Schrödinger Equation, you may find the following blog post and examples useful:

https://www.comsol.com/blogs/computing-the-band-gap-in-superlattices-with-the-schrodinger-equation/

https://www.comsol.com/model/double-barrier-1d-47041

https://www.comsol.com/model/superlattice-band-gap-tool-45281

Tutorial Model: DC Characteristics of a MOSFET

This tutorial calculates the DC characteristics of a MOS (metal–oxide–semiconductor) transistor. The MOSFET (metal oxide semiconductor field-effect transistor) is by far the most common semiconductor device, and the primary building block in all commercial processors, memories, and digital integrated circuits. Since the first microprocessors were introduced approximately 40 years ago this device has experienced tremendous development, and today it is being manufactured with feature sizes of 22 nm and smaller.

The MOSFET is essentially a miniaturized switch. In this example the source and drain contacts (the input and output of the switch) are both ohmic (low resistance) contacts to heavily doped n-type regions of the device. Between these two contacts is a region of p-type semiconductor. The gate contact lies above the p-type semiconductor, slightly overlapping the two n-type regions. It is separated from the semiconductor by a thin layer of Silicon oxide, so that it forms a capacitor with the underlying semiconductor. Applying a voltage to the gate changes the local band structure beneath it through the Field Effect. A sufficiently high voltage can cause the semiconductor to change from p-type to n-type in a thin layer (the channel) underneath the gate. This is known as inversion and the channel is sometimes referred to as the inversion layer. The channel connects the two n-type regions of semiconductor with a thin n-type region under the gate. This region has a significantly lower resistance than the series resistance of the n–p/p–n junctions that separated the source and the drain before the gate voltage produced the inversion layer. Consequently, applying a gate voltage can be used to change the resistance of the device. The gate voltage where a significant current begins to flow is called the threshold or turn-on voltage. Figure 7 shows a schematic MOSFET with the main electrical connections highlighted. Figure 8 shows an electron microscope image of a modern MOSFET device.
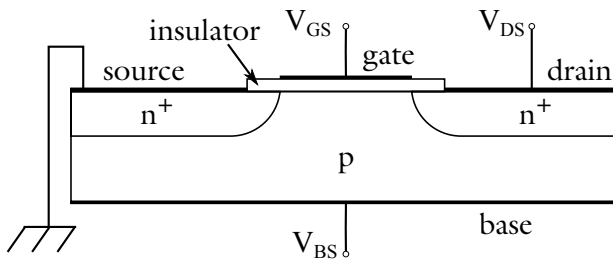
Figure 7: Schematic diagram of a typical MOSFET. The current flows from the source to the drain through a channel underneath the gate. The size of the channel is controlled by the gate voltage.
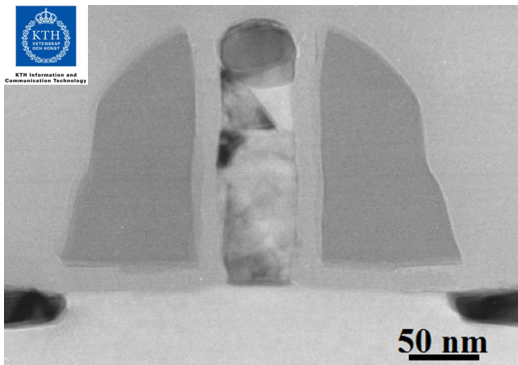
Figure 8: Cross-section TEM (transmission electron microscopy) image of a 50 nm gate length MOSFET fabricated at KTH Electrum laboratory by P.E Hellström and coworkers within the ERC advanced grant OSIRIS research project headed by Prof. M. Östling.

As the voltage between the drain and the source is increased the current carried by the channel eventually saturates through a process known as pinch-off, in which the channel narrows at one end due to the effect of the field parallel to the surface. The channel width is controlled by the gate voltage. Typically a larger gate voltage results in wider channel and consequently a lower resistance for a given drain voltage. Additionally, the saturation current is larger for a higher gate voltage.
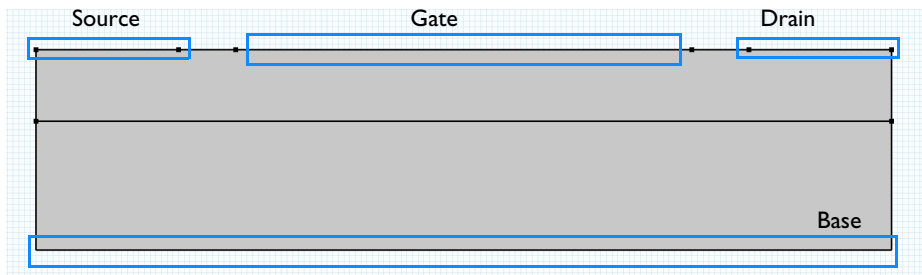
Figure 9: Model geometry showing the external connections.

Figure 9 shows the model geometry, indicating how the geometry elements correspond to features in Figure 7. In this model both the source and the base are connected to ground and the voltages applied to the drain and the gate are varied. In the first study a small voltage (10 mV) is applied to the Drain and the Gate voltage is swept from 0 to 5 V. A plot of the current flowing between the source and the drain is used to determine the turn-on voltage of the device. The second study sweeps the drain voltage from 0 to 5 V at three different values of the gate

voltage (2, 3, and 4 V). The drain current versus drain voltage is then plotted at several values of the gate voltage.

Model Wizard

Note: These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and Mac.

1 To start the software, double-click the COMSOL icon on the desktop. When the software opens, you can choose to use either the Model Wizard to create a new model, or Blank Model to create one manually. For this tutorial, click the Model Wizard button.

If COMSOL Multiphysics is already open, you can start the Model Wizard by selecting New from the File menu and then click Model Wizard .

The Model Wizard guides you through the first steps of setting up a model. The next window lets you select the dimension of the modeling space.

2 In the Select Space Dimension window, click the 2D button .

3 In the Select Physics tree, under the Semiconductor branch, click Semiconductor (semi) .

4 Click Add button. Observe that the Semiconductor interface is added in the "Added physics interfaces" pane. Click the Study button .

5 In the Select Study tree, under General Studies branch, click Stationary .

6 Click Done .

Global Definitions

Parameters

1 On the Home ribbon/toolbar click Parameters P_i and select Parameters 1 P_i .

Note: On Linux and Mac, the Home ribbon/toolbar refers to the specific set of controls near the top of the Desktop.

2 In the Settings window for Parameters, locate the Parameters section. In the table, enter the following settings:

NAME	EXPRESSION	DESCRIPTION
Vd	10[mV]	Drain Voltage
Vg	2[V]	Gate Voltage

These are examples of global parameters that we can use to parameterize the model. The parameters can be any global quantity, such as the geometric dimensions, material properties, or doping concentrations, just to name a few.

Geometry 1

The geometry can be specified using the built-in tools in COMSOL Multiphysics. First choose to define geometry objects using micrometer units.

1 In the Model Builder tree, under Component 1, click Geometry 1 ⚠.

2 In the Settings window for Geometry, locate the Units section. From the "Length unit" list (drop-down menu), choose μm.

Rectangle 1

Next create a rectangle to define the geometry extents.

1 In the Model Builder, right click Geometry 1 ⚠ and choose Rectangle ▭.

2 In the Settings window for Rectangle, locate the "Size and Shape" section. In the Width text field, type 3. In the Height text field, type 0.7.

Polygon 1

Add a polygon that includes points to define the source, drain, and gate contacts. It will also include a line to help create the mesh.

1 Right click Geometry 1 ⚠, hover over "More Primitives" to open the submenu and choose Polygon ⟋.

2 In the Settings window for Polygon, locate the Object Type section. From the Type list, choose "Closed curve".

3 Locate the Coordinates section. From the "Data source" list, select Table.

- In the x text field, type 0 0 0.5 0.7 2.3 2.5 3 3.
- In the y text field, type 0.67 0.7 0.7 0.7 0.7 0.7 0.7 0.67.

▼ Coordinates

Data source: Table

x (µm)	y (µm)
0	0.67
0	0.7
0.5	0.7
0.7	0.7
2.3	0.7
2.5	0.7
3	0.7
3	0.67

Polygon 1

1 On the Geometry ribbon/toolbar, click Virtual Operations 🐌 and choose Mesh Control Edges ⬡.

2 In the Settings window for Mesh Control Edges, locate the Input section. For the "Edges to include:" input panel, select Boundary 4 (the interior line that was just created by the Polygon step). This tells the software that Boundary 4 is used for mesh generation only, and is ignored by the physics settings.
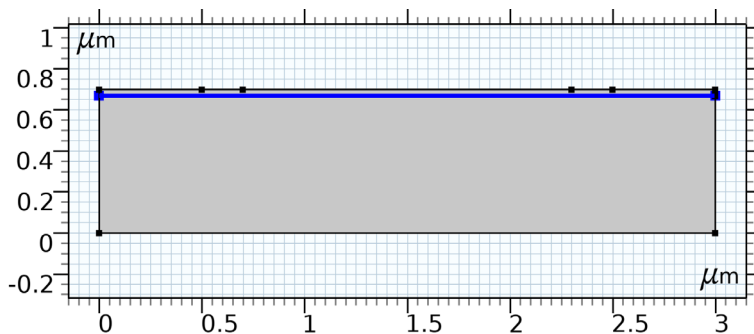
3 Click the Build All button ▦ to build the entire geometry. Use the Zoom Extents button ⊹ at the top of the Graphics window to zoom to the full geometry if desired. Notice that the interior line is not shown in the finalized geometry, because it is defined as a Mesh Control Edge in the previous step and will only appear when we set up the mesh later.

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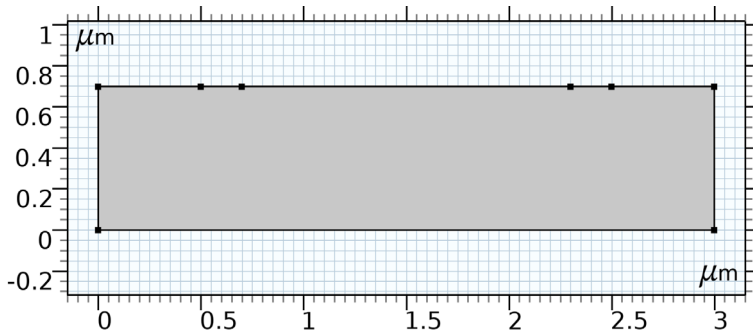
Materials

Add Material

Next the material properties are added to the model.

1 On the Home ribbon/toolbar click Add Material ⬛.

2 Go to the Add Material window. In the tree, under the Semiconductors branch, click Si ⬛.

3 Click ➕ Add to Component.

4 On the Home ribbon/toolbar click Add Material ⬛ to close the Add Material window.

Semiconductor

Next define the physics settings. Start with the carrier statistics and doping.

1 In the Model Builder window, click Semiconductor ⬛.

2 In the Settings window for Semiconductor, locate the Model Properties section. From the "Carrier statistics" list, choose Fermi–Dirac.

Analytic Doping Model 1

First a constant background acceptor concentration is defined.

1 On the Physics ribbon/toolbar, click the Domains menu and choose Analytic Doping Model ⬤.
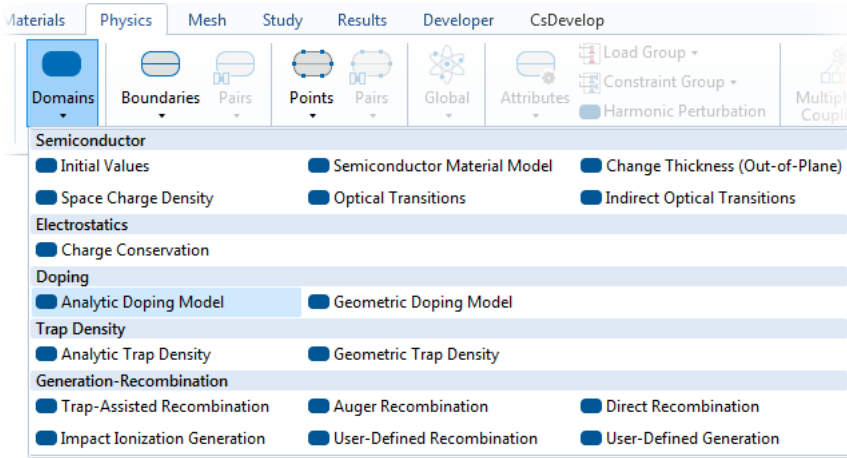
2 In the Settings window for Analytic Doping Model locate the Domain Selection section. From the Selection list, choose All domains.

3 Locate the Impurity section. In the N_{A0} text field, type `1e17[1/cm^3]`.

Analytic Doping Model 2

Add a second doping feature to define the implanted doping profile for the source.

1 On the Physics ribbon/toolbar click the Domains menu and choose Analytic Doping Model ⬤.

2 In the Settings window for Analytic Doping Model, locate the Domain Selection section. From the Selection list, choose All domains.

3 Locate the Distribution section. From the list, choose Box.

When defining a Box doping distribution, a rectangular region of constant doping is defined, with a Gaussian drop off away from the edges of this rectangular region.

Define the location of the lower-left corner of the uniformly doped rectangular region.

1 Locate the Uniform Region section.

  - Specify the Base position: r_0 vector as

0[um]	X
0.6[um]	Y

2 Then define the width and height of the uniformly doped region.

  - In the Width: W text field, type `0.6[um]`.
  - In the Depth: D text field, type `0.1[um]`.

Choose the dopant type and the doping level in the uniformly doped region.

3 Locate the Impurity section.

  - From the "Impurity type" list, choose "Donor doping (n-type)".
  - In the N_{D0} text field, type `1e20[1/cm^3]`.

Next, specify the length scale over which the Gaussian drop off occurs. If doping into a background dopant distribution of opposite type (as in this case), this setting specifies the junction depth. In this model, different length scales are used in the x and y directions.

4 Locate the Profile section. Select the "Specify different length scales for each direction" checkbox.

5 Specify the d_j vector as

0.2[um]	X
0.25[um]	Y

Finally specify the constant background doping level.

6 From the N_b list, choose "Acceptor concentration (semi/adm1)".

7 You can visualize doping profiles by clicking the preview buttons before solving the model. Two buttons named as [icon] Plot Doping Profile for Selected and [icon] Plot Net Doping Profile for All are available both in the toolbar and the context menu. The doping profile will be shown in a separate plot window named as [icon]

Doping Profile Plot. Note that p-type and n-type domains are shown in red and blue color, respectively.
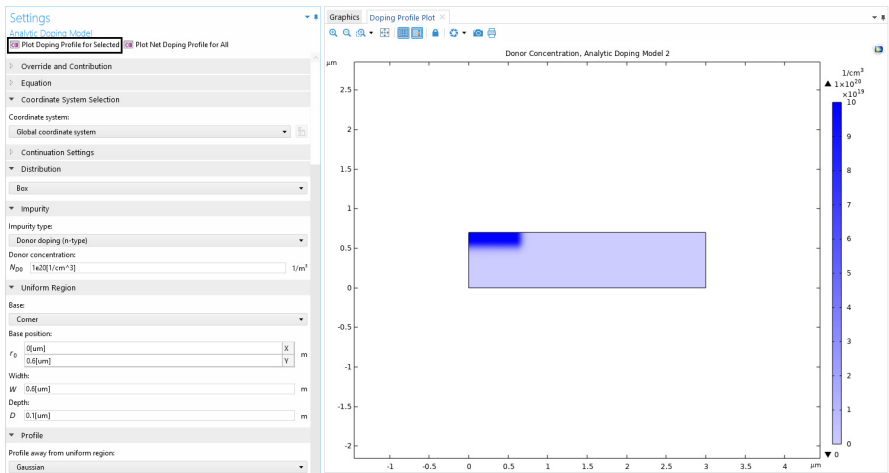
Analytic Doping Model 3

Add a similar Gaussian doping profile for the drain.

1 Right-click Analytic Doping Model 2 and choose Duplicate 🔁 .

2 In the Settings window for Analytic Doping Model, locate the Uniform Region section.

- Specify the r_0 vector as

2.4[um]	X
0.6[um]	Y

Next set up boundary conditions for the contacts and gate.

Metal Contact 1

First add a contact for the source.

1 On the Physics ribbon/toolbar click the Boundaries menu and choose Metal Contact ⊖ .

The Metal Contact feature is used to define Metal–Semiconductor interfaces of various types. In this instance use the default Ideal Ohmic contact type to define the source.

2 Select Boundary 3 only.
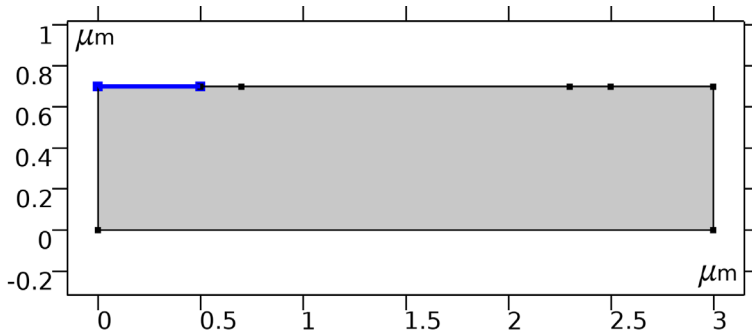
Note: The Metal Contact feature in COMSOL Multiphysics is a so called Terminal boundary condition. By default a fixed potential of 0 V is applied, which is appropriate in this instance, since the source is grounded. The terminal can also be set up to specify an input current, input power, or to connect to a voltage or current source from an external circuit.

Metal Contact 2

Add a second Metal Contact feature to define the drain.

1 On the Physics ribbon/toolbar click the Boundaries menu and choose Metal Contact ⬭.

2 Select Boundary 7 only.
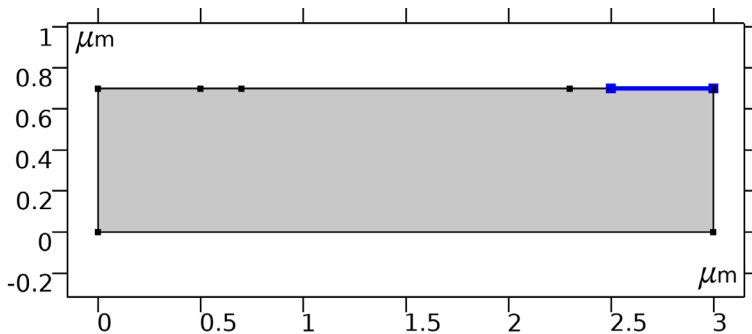
Set the drain voltage to be specified by the previously defined parameter.

3 In the Settings window for Metal Contact, locate the Terminal section. In the V_0 text field, type vd.

Metal Contact 3

Add a third Metal Contact to set the body voltage to 0 V.

1 On the Physics ribbon/toolbar click the Boundaries menu and choose Metal Contact ⬭.

2 Select Boundary 2 only.
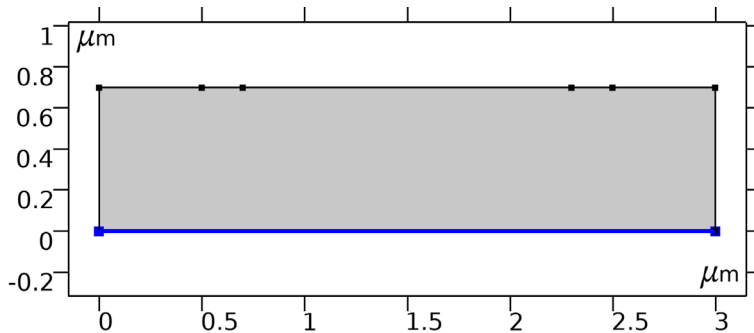
Thin Insulator Gate 1

Set up the Gate. The Gate dielectric is not explicitly represented in the model, instead the Thin Insulator Gate boundary condition represents both the gate contact and the thin layer of oxide.

1 On the Physics ribbon/toolbar click the Boundaries menu and choose Thin Insulator Gate ⬭.

The Thin Insulator Gate feature is also a terminal, but in this instance it is possible to fix the voltage or charge on the terminal, as well as to connect it to a circuit.

Note: The charge setting determines the charge on the conductor and does not relate to trapped charge at the oxide–semiconductor interface.

The voltage applied to the gate is specified by the parameter added previously.

2 In the Settings window for Thin Insulator Gate, locate the Terminal section. In the V_0 text field, type Vg.

3 Locate the Gate Contact section.

- In the ε_{ins} text field, type 4.5.
- In the d_{ins} text field, type 30[nm].

4 Select Boundary 5 only.
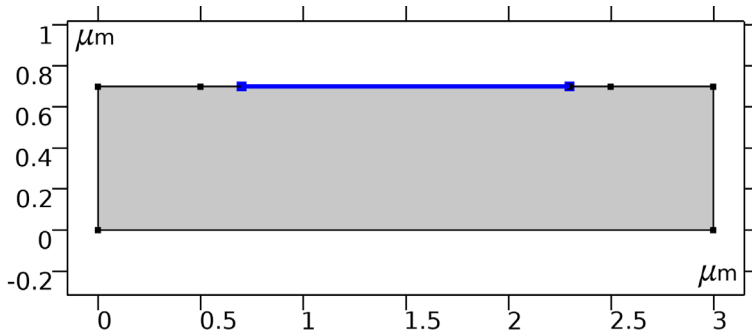
Trap-Assisted Recombination 1

A range of generation–recombination mechanisms are available to be added to the model. In this case, we simply add trap-assisted recombination, using the default Shockley–Read–Hall model.

1 On the Physics ribbon/toolbar click the Domains menu and choose Generation–Recombination section > Trap-Assisted Recombination ●.

2 In the Settings window for Trap-Assisted Recombination, locate the Domain Selection section. From the Selection list, choose All domains.

Mesh 1

We will use a user-defined mesh for this model.

1 In the Model Builder window, under Component 1 (comp1) click Mesh 1 △.

2 In the Settings window for Mesh, locate the Mesh Settings section. From the "Sequence type" 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. Click the Custom button.

3 Locate the Element Size Parameters section. In the "Maximum element growth rate" text field, type 1.05.

1 In the Model Builder window, under Component 1 (comp1) > Mesh 1 right-click Size 1 ◮ and choose Delete. In the Confirm Delete pop-up window, click Yes.

2 Right-click Size 2 ◮ and choose Delete. In the Confirm Delete pop-up window, click Yes.

3 Right-click Free Triangular 1 ◭ and choose Delete. In the Confirm Delete pop-up window, click Yes.

Edge 1

1 Right-click Mesh 1 and choose Edge ◮.

2 In the Settings window for Edge, locate the "Boundary Selection" section. Select Boundaries 3–7 only (the top surface of the device).
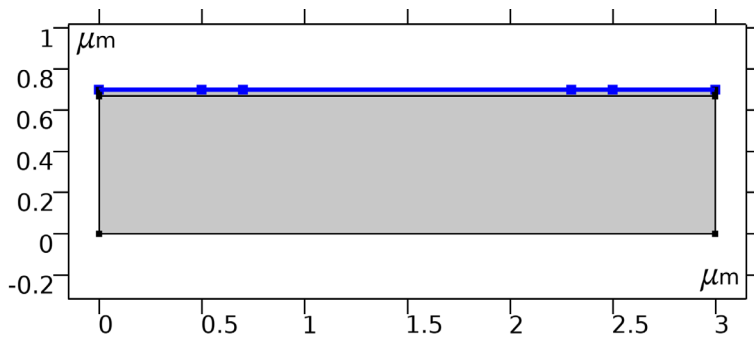
3 Click to expand the "Control Entities" section. Clear the "Smooth across removed control entities" checkbox.

Size 1

1 Right-click Edge 1 and choose Size ◮.

2 In the Settings window for Size, locate the Element Size section.

  - From the "Calibrate for" list, choose Semiconductor.

  - Click the Custom button.

3 Locate the Element Size Parameters section.

  - Select the "Maximum element size" checkbox.

  - In the associated text field, type 0.03.

Mapped 1

1 In the Model Builder window, right-click Mesh 1 and choose Mapped ⬚.

2 In the Settings window for Mapped, locate the Domain Selection section.

- From the "Geometric entity level" list, choose Domain.
- Select Domain 2 only.
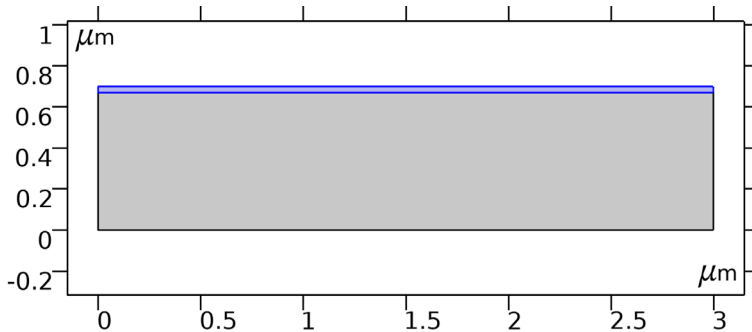
3 Click to expand the "Control Entities" section. Clear the "Smooth across removed control entities" checkbox.

4 Click to expand the Reduce Element Skewness section. Select the "Adjust edge mesh" checkbox.

Distribution 1

1 Right-click Mapped 1 and choose Distribution ▦.

2 Select Boundary 9 only (use the mouse scroll wheel to cycle through possible selections when multiple ones are within a short distance from the mouse pointer, as in this case).
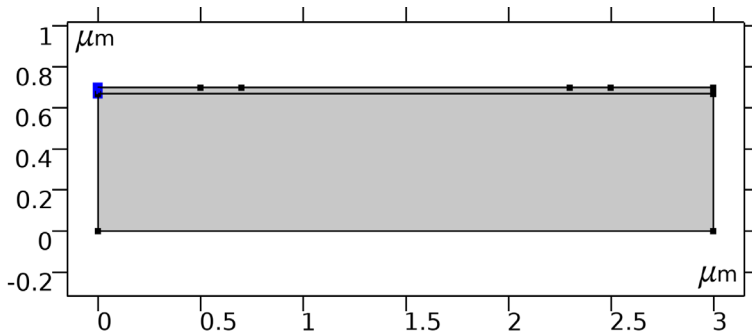
3 In the Settings window for Distribution, locate the Distribution section.

- From the "Distribution type" list, choose Predefined.
- In the "Number of elements" text field, type 8.
- In the "Element ratio" text field, type 9.
- From the "Growth rate" list, choose "Exponential".
- Select the "Reverse direction" checkbox.

Free Triangular 1

1 In the Model Builder window, right-click Mesh 1 and choose Free Triangular ▨ .

2 In the Settings window for Free Triangular, click to expand the "Control entities" section. Clear the "Smooth across removed control entities" checkbox.

3 Click Build all ▦ .

The user-defined mesh is shown in the images below. The mapped mesh with the specific distribution helps create layers of thin elements underneath the gate, where the large gradient of the carrier concentration needs to be resolved by the mesh.
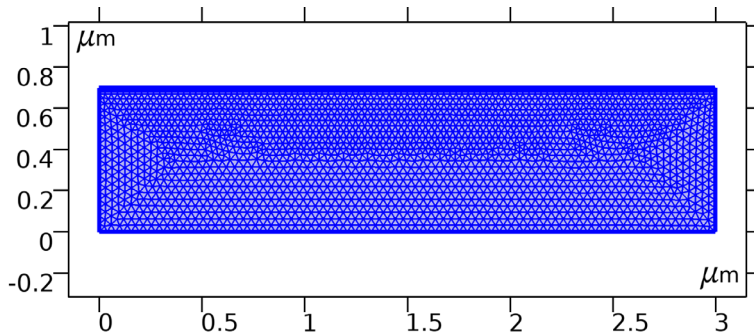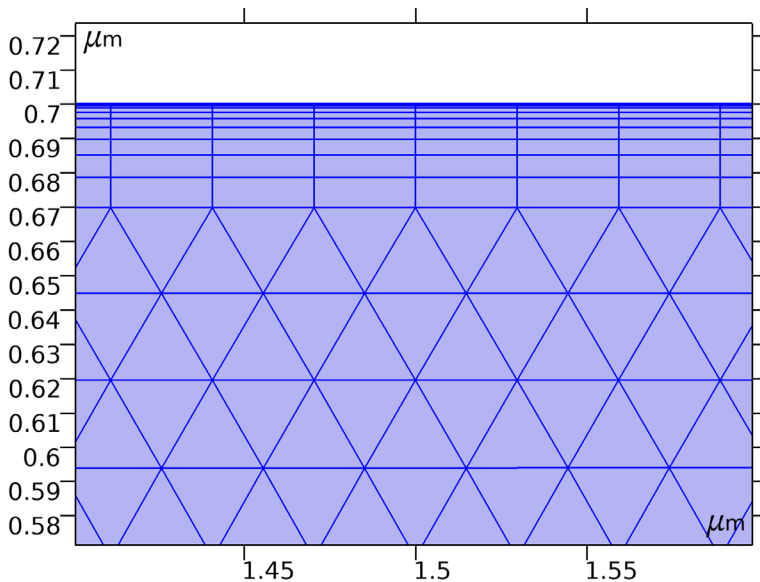
Study 1

Before setting up the study, check that the doping was set up correctly. To do this, first get the initial value for the study.

1 In the Model Builder click Study 1 ∞.

Disable the default plots since these are not required.

2 In the Settings window for Study locate the "Study Settings" section. Click to clear the "Generate default plots" checkbox.

**3** On the Study ribbon/toolbar click Get Initial Value $\frac{U}{t=o}$.

Results

2D Plot Group 1

Add a 2D plot group to check the dopant distribution in the model.

1 On the Home ribbon/toolbar click Add Plot Group 🗐 and choose 2D Plot Group ■.

2 Rename the Plot Group by typing "Signed Dopant Concentration" in the Label field.

3 On the Signed Dopant Concentration ribbon/toolbar click Surface ■.

Plot the signed dopant concentration (Nd–Na). This quantity is positive for net donor doping and negative for net acceptor doping.

4 In the Model Builder under Results > Signed Dopant Concentration, click Surface 1 ■.

5 In the Settings window for Surface, locate the Expression section. In the Expression text field, type `semi.Nd-semi.Na`.

6 Change the Unit field under Expression from 1/m^3 to 1/cm^3

7 Click the Plot button ⊡.

The doping distribution is shown below.
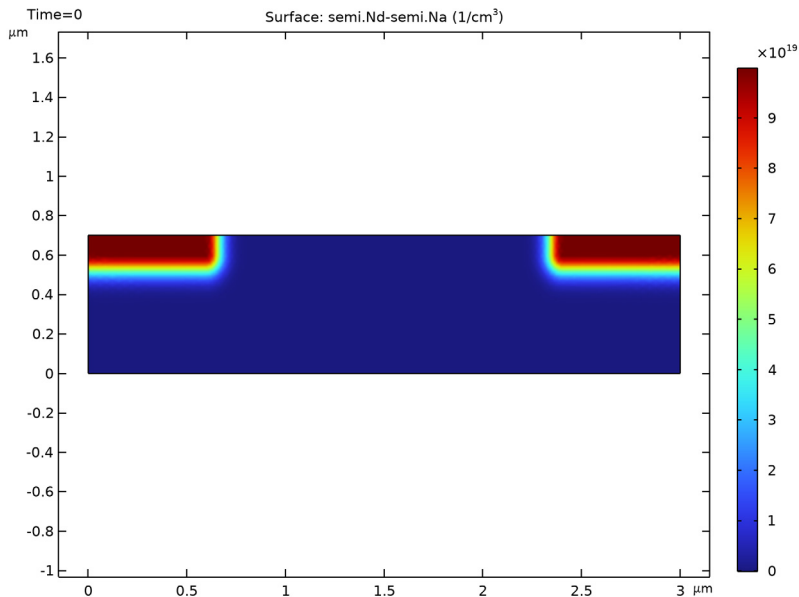
Study 1

Step 1: Stationary

Now set up a Stationary study to determine the turn-on voltage for the transistor. In this study we set Vd to 10 mV and sweep over Vg.

1 In the Model Builder under Study 1, click Step 1: Stationary ⬚ .

2 In the Settings window for Stationary click to expand the "Study Extensions" section.

The study extensions panel can be used to set up a parametric sweep.

3 Under the "Study Extensions" section, select the "Auxiliary sweep" checkbox.

4 From the "Sweep type" list, choose "All combinations". This option sweeps over every combination of the specified parameters.

5 Click Add ＋ . In the table, enter the following settings:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
Vd	0.01	V

The drain voltage is fixed at a constant value of 10 mV.

6 Click Add ＋ again to add Vg to the table.

7 In the table cell for the parameter value list for Vg, enter `range(0,0.2,1.4)` 2 3 4. This sweeps the gate voltage between 0 and 4V with uneven step sizes, to reduce computation time and file size.

By default the "Run continuation for" setting is set to "Last parameter" (Vg in this case). This setting configures the solver to use the solution for the previous value of Vg as the initial guess for the solution when solving for the next value of Vg. It also allows the solver to take intermediate steps at values of Vg not specified in the parameter value list if necessary. Using this continuation option is a standard technique to achieve convergence for highly nonlinear equation systems such as the semiconductor equation system.

8 On the Home ribbon/toolbar click Compute ＝ .

Results

1D Plot Group 2

Add a 1D plot group to plot the source current versus the gate voltage.

1 On the Home ribbon/toolbar click Add Plot Group 🔲 and choose 1D Plot Group ∿ .

2 Rename the Plot Group by typing "Id vsVg (Vd=10mV)" in the Label field.

3 On the "Id vsVg (Vd=10mV)" ribbon/toolbar click Global ⊝ .

The postprocessing menus contain a wide range of quantities available for plotting. Choose the current flowing into terminal 2.

4 In the Settings window for Global ⟳ click Replace Expression ⊟▾ (it is in the upper-right corner of the "y-Axis Data" section — do not get confused with the same button for the "x-Axis Data"). In the menu, expand the tree to Model > Component1 > Semiconductor > Terminals, and then double click "semi.I0_2 - Terminal Current - A".

5 Change the Unit to uA and click the Plot button ⊡ .

Global: Terminal current (uA)
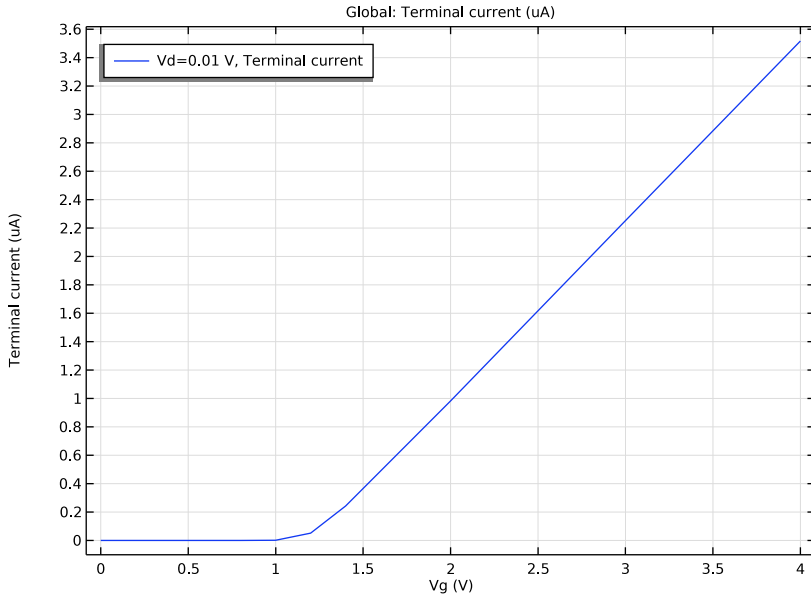
From the plot it is clear that the threshold voltage, V_T, of the transistor is approximately 1.2 V. It is possible to compare this value with the theoretical value given by (S. M. Sze and K. K. Ng, *Physics of Semiconductor Devices*, Wiley, Hoboken, New Jersey, pp. 305–306, 2007):

$$V_T \cong V_{FB} + 2\psi_B + \frac{d_{ox}(4\varepsilon_{r,s}\varepsilon_0 q N_a \psi_B)^{\frac{1}{2}}}{\varepsilon_{r,ox}\varepsilon_0}$$

where d_{ox} is the thickness of the oxide and $\varepsilon_{r,ox}$ is its relative permittivity, ε_0 is the permittivity of free space, $\varepsilon_{r,s}$ is the relative permittivity of the semiconductor, q is the electron charge and N_a is the acceptor concentration under the gate. The flat band voltage V_{FB} and the potential difference between the intrinsic level and the Fermi-level, Ψ_B, are given by the following equations:

$$V_{FB} = \Phi_m - \chi + \frac{k_B T}{q} \ln\left(\frac{n_{eq}}{N_c}\right)$$

$$\psi_B = \frac{k_B T}{q} \ln\left(\frac{p_{eq}}{n_i}\right)$$

where Φ_m is the work function of the metal contact, χ is the semiconductor electron affinity, k_B is Boltzmann's contact, T is the absolute temperature, N_c is the semiconductor density of states in the conduction band and n_i is the intrinsic carrier density. The equilibrium electron (n_{eq}) and hole (p_{eq}) densities are given by:

$$n_{eq} = \frac{1}{2}(N_d - N_a) + \frac{1}{2}\sqrt{(N_d - N_a)^2 + 4n_i}$$

$$p_{eq} = -\frac{1}{2}(N_d - N_a) \pm \frac{1}{2}\sqrt{(N_d - N_a)^2 + 4n_i}$$

Where N_d is the donor concentration under the gate. Note that these equations assume both complete ionization and Maxwell Boltzmann statistics (reasonable assumptions near the threshold condition). These equations give a threshold voltage of 1.18 V, in good agreement with the simulation result. Follow the steps below to compute the threshold voltage using the approximate formulas above.

Variables 1

1 In Model Builder, right-click Component 1 > Definitions, select Variables a= .

2 In the Settings window for Variables, under the Geometric Entity Selection section, for the "Geometric entity level" list, select Point. Then select Point 4.
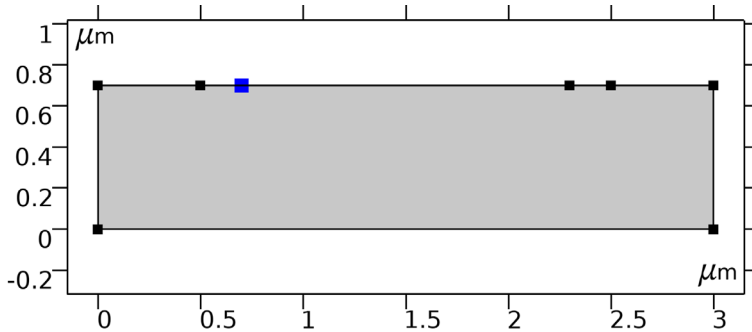
3 In the Settings window for Variables, under the Variables section, enter the Name and Expression of the three variables:

NAME	EXPRESSION
VFB	`semi.Phi-semi.chi_semi+semi.Vth*log(semi.ni^2/semi.Na/semi.Nc)`
PsiB	`semi.Vth*log(semi.Na/semi.ni)`
VT	`VFB+2*PsiB+semi.d_ins*sqrt(4*semi.epsilonrs*e_const*` `semi.Na*PsiB/epsilonO_const)/semi.epsilon_ins`

Study 1

4 In the Model Builder, right-click Study 1, select Update Solution ⟳ .

This allows the solution to recognize the three variables that we just defined, without having to recompute the study.

Results

5 In the Model Builder, right-click Results, select Evaluation Group. 🗒

Evaluation Group 1

6 In the Settings window for Evaluation Group, under the Data section, for the two lists "Parameter selection (Vd)" and "Parameter selection (Vg)", select First, since the evaluation of the threshold voltage is independent of the drain or gate voltage.

7 In the Model Builder, right-click Results > Evaluation Group 1, select Point Evaluation.

Point Evaluation 1

8 In the Settings window for Point Evaluation, under the Selection section, select Point 4 only.
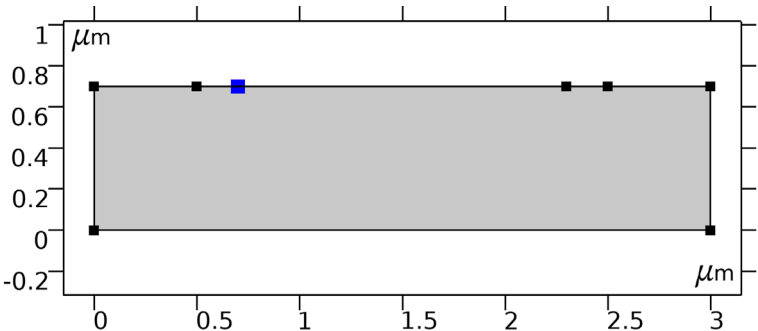
9 Under the Expressions section, enter the three variable names `VFB`, `PsiB`, and `VT` into the Expression column of the table.

10 Click Evaluate.

The results are -0.95 V, 0.43 V, and 1.18 V, respectively.

Study 2

Now add an additional study to plot the source current as a function of drain voltage at a range of different gate voltages.

1 On the Home ribbon/toolbar click Add Study ∞.

2 In the Add Study window, find the Studies subsection. In the tree under General Studies, click Stationary ⟋.

3 Click Add Study ╋ in the window toolbar.

4 On the Home ribbon/toolbar click Add Study ∞ to close the Add Study window.

Step 1: Stationary

1 In the Model Builder under Study 2, click Step 1: Stationary ⟋.

2 In the Settings window for Stationary locate the Study Extensions section.

3 Select the Auxiliary sweep checkbox.

4 From the "Sweep type" list, choose "All combinations".

5 Click Add ╋ . Select Vg from the Parameter name list.

Now set up the study to sweep over Vg.
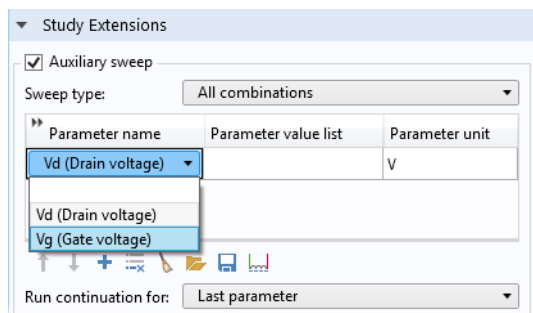
6 Click Range . Go to the Range dialog.

 - In the Start text field, type 2.
 - In the Step text field, type 1.
 - In the Stop text field, type 4.

7 Click Replace.

8 Click Add ╋ . In this case the default Auxiliary Parameter Vd is the desired parameter for the sweep.

9 In the table cell for the parameter value list for Vd, enter
`range(0,0.25,1.5) 2 3 4 5`.

The *inner* sweep over Vd, the last parameter, should be used for the continuation solver (this is the default), since the solution will only change slightly between close values of Vd.

Configure the solver to reuse the solution from the previous step of the continuation parameter sweep as the initial value for the next step for the *outer* sweep parameter Vg, using the first value of the *inner* parameter Vd

10 From the "Reuse solution for previous step" list, choose Auto.

11 On the Home ribbon/toolbar click Compute $=$.

Results

By looking at the electron concentration at Vd values of 0, 1, and 5 V the pinch-off of the channel can be clearly seen.

Electron Concentration (semi)

1 In the Model Builder under Results, click Electron Concentration (semi) ▪ .

By default the plot shows the results for the case Vg=4 V and Vd=5 V.

2 In the Settings window for 2D Plot Group locate the Data section. Change the Vd Parameter value to 1 V and then to 0 V, each time selecting the Plot button ▭ to see how the results change.

Electric Potential (semi)

1 In the Model Builder under Results, click Electric Potential (semi) ▪ .

2 Look at the plot for Vd values of 5 V, 1 V and 0 V.

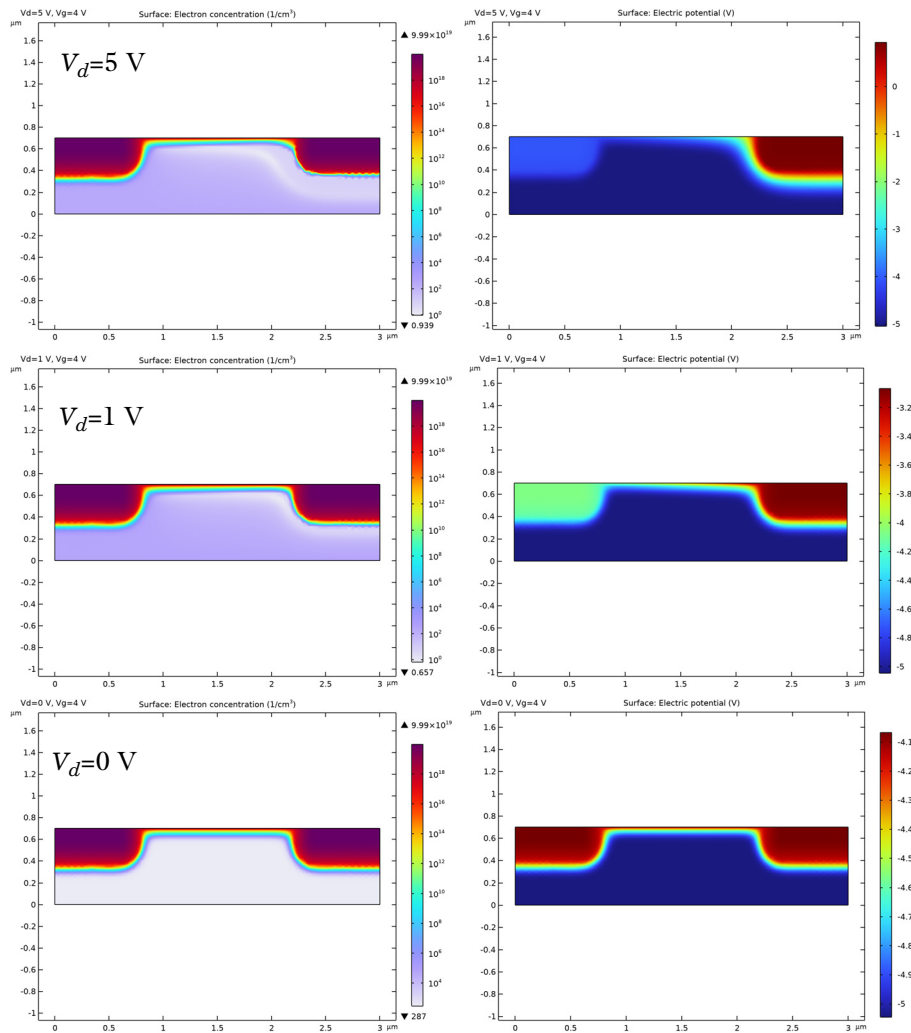The plots in Figure 10 show the results. The pinch off effect is apparent at 5 V.

Figure 10: Electron concentration and electric potential distribution at Vd values of 0, 1, and 5 V. The pinch-off of the channel is apparent at 5 V.

Add another 1D plot group to plot the drain current versus the drain voltage.

3 On the Home ribbon/toolbar select Add Plot Group 🖼, and choose 1D Plot Group ∿.

4 Rename the plot group by typing "Id vs. Vd" in the Label field.

5 In the Settings window for 1D Plot Group locate the Data section. From the "Dataset" list, choose Study 2/Solution 2.

1D Plot Group 6

1 From the "Id vs. Vd" ribbon/toolbar click Global ⊕.

2 In the Model Builder under Results > Id vs. Vd, click Global 1 ⊕.

3 In the Settings window for Global click Replace Expression ▭▾ in the upper-right corner of the "y-Axis Data" section. In the menu, expand the tree to Model > Component1 > Semiconductor > Terminals, and then double click "semi.I0_2 - Terminal Current - A".

4 Change the Unit to uA for the current.

5 Click the Plot button ▣.
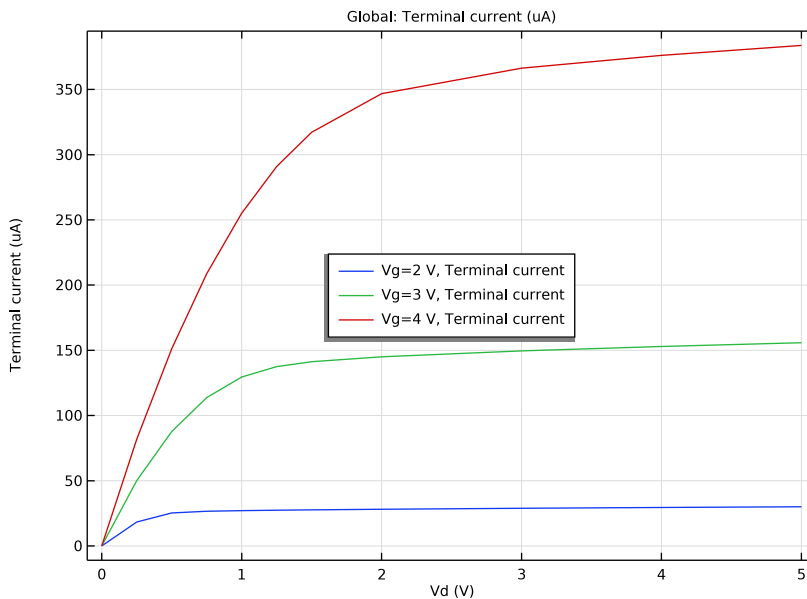
The drain current versus drain voltage diagram shows a linear region for low bias, followed by a nonlinear region. The drain current increases slightly with voltage in the saturation region at higher drain voltages, as a result of short channel effects. Short channel effects mean that the standard analytic expressions for the saturation voltage and current do not apply, but the saturation voltages and currents are of a similar magnitude to those predicted by the simple theory (S.M. Sze and K.K. Ng, *Physics of Semiconductor Devices*, Wiley, Hoboken, New Jersey, pp. 305–306, 2007).