

Electric Discharge Module

User's Guide

Electric Discharge Module User's Guide

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Introduction

This guide describes the Electric Discharge Module, an optional add-on package for COMSOL Multiphysics® designed to assist you to solve and model electric discharges.

This chapter introduces you to the capabilities of the module including an introduction to the modeling stages and some realistic and illustrative models. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

In this chapter:

- [About the Electric Discharge Module](#)
- [Overview of the User's Guide](#)

About the Electric Discharge Module

In this section:

- [What Can the Electric Discharge Module Do?](#)
- [Electric Discharge Module Physics Interface Guide](#)
- [Common Physics Interface and Feature Settings and Nodes](#)
- [Where Do I Access the Documentation and Application Libraries?](#)

What Can the Electric Discharge Module Do?

The Electric Discharge Module provides a unique environment for simulation of electric discharges. The module is a powerful tool for detailed analysis of low-temperature and high-temperature gas discharges as well as charge transport in liquid and solid dielectrics. With this module you can run static and transient simulations in an easy-to-use user interface.

The available physics interfaces cover the following types of electric discharge simulations:

- Arc discharges
- Corona discharges
- Dielectric barrier discharges
- Electrostatic discharges
- Streamer discharges

In addition to the standard results and visualization functionality, the module supports direct computation of lumped parameters such as discharge current.

Selected material data are provided with the module.



For detailed information about [Materials](#) including the [Electric Discharge Material Library](#), see the *COMSOL Multiphysics Reference Manual*.

Like all COMSOL modules, there is a library of ready-to-run models that make it quicker and easier to analyze discipline-specific problems. In addition, any model you develop is described in terms of the underlying partial differential equations, offering a unique way to see the underlying physical laws of a simulation.

The Electric Discharge interfaces are fully multiphysics enabled — couple them to any other physics interface in COMSOL Multiphysics or other modules. The Electric Discharge Module contains predefined multiphysics interfaces to facilitate easy setup of models with the most commonly occurring couplings. For example, the Arc Discharge multiphysics interface combines all features from the Magnetic and Electric Fields interface in the stationary and time-dependent formulations with the Heat Transfer interface and Laminar Flow interface to model the dynamics of electric arc. The Electric Discharge Module also provides interfaces for modeling electrical circuits.



- [Building a COMSOL Multiphysics Model](#) in the *COMSOL Multiphysics Reference Manual*
- [Electric Discharge Module Physics Interface Guide](#)
- [Common Physics Interface and Feature Settings and Nodes](#)
- [Where Do I Access the Documentation and Application Libraries?](#)














Electric Discharge Module Physics Interface Guide





The interfaces in the Electric Discharge Module form a complete set of simulation tools for electric discharge simulations. To select the right physics interface for describing the real-life physics, the geometric properties and the time variations of the fields need to be considered.

Each physics interface has a *tag*, which is of special importance when performing multiphysics simulations. This tag helps distinguish between physics interfaces and the variables defined by the physics interface have an underscore plus the physics interface tag appended to their names.

The *Model Wizard* is an easy way to select the physics interface and study type when creating a model for the first time, and physics interfaces can be added to an existing model at any time. Full instructions for selecting interfaces and setting up a model are in the *COMSOL Multiphysics Reference Manual*.

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		es	all dimensions	stationary; time dependent; stationary source sweep; eigenfrequency; frequency domain; small signal analysis, frequency domain
Magnetic and Electric Fields		mef	3D, 2D, 2D axisymmetric	stationary; time dependent
 Chemical Species Transport				
Chemistry		chem	all dimensions	stationary; time dependent
Reaction Engineering		re	0D	time dependent; stationary plug flow
 Electric Discharge				
Electric Discharge		edis	all dimensions	time dependent; stationary; frequency domain perturbation
Arc Discharge		—	all dimensions	time dependent; stationary; frequency-transient; frequency-stationary
Transport of Charge Carriers		tcc	all dimensions	time dependent; stationary; frequency domain perturbation
 Plasma				
Corona Discharge		—	all dimensions	stationary

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Electrical Breakdown Detection		ebd	3D, 2D, 2D axisymmetric	time dependent
 Radio Frequency				
Electromagnetic Waves, Transient		temw	3D, 2D, 2D axisymmetric	eigenfrequency; time dependent; time dependent, modal; time dependent with FFT
Transmission Line, Transient		tlt	3D, 2D, 1D	time dependent

In 2D, in-plane and out-of-plane variants are available for problems with a planar symmetry as well as axisymmetric interfaces for problems with a cylindrical symmetry.



When using an axisymmetric physics interface it is important that the horizontal axis represents the r direction and the vertical axis the z direction, and that the geometry in the right half plane (that is, for positive r only) must be created.

See [What Problems Can You Solve?](#) for information about the available study types and variables. See also [Overview of the User's Guide](#) for links to the chapters in this guide.




In the *COMSOL Multiphysics Reference Manual*:

- [Studies and Solvers](#)
- [The Physics Interfaces](#)
- For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see [Physics Interface Guide](#).

Common Physics Interface and Feature Settings and Nodes


There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used.

In each module’s documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

	In the <i>COMSOL Multiphysics Reference Manual</i> see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the Help window or Ctrl+F1 to open the Documentation window.
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Where Do I Access the Documentation and Application Libraries?

A number of online resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the Application Libraries are all accessed through the COMSOL Desktop.

	If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.
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COMSOL Blog	www.comsol.com/blogs
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COMSOL Application Gallery	www.comsol.com/models
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Learning Center	www.comsol.com/support/learning-center
Support Knowledge Base	www.comsol.com/support/knowledgebase

Overview of the User's Guide

The *Electric Discharge Module User's Guide* gets you started with modeling using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions how to use COMSOL in general are included with the *COMSOL Multiphysics Reference Manual*.



As detailed in the section [Where Do I Access the Documentation and Application Libraries?](#) this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS, GLOSSARY, AND INDEX

To help you navigate through this guide, see the [Contents](#), [Glossary](#), and [Index](#).

MODELING GUIDELINES

The [Modeling Guidelines](#) chapter summarizes general procedures and strategies for modeling electric discharges. Topics include [Connecting to Electrical Circuits](#), [SPICE Import and Export](#), [Meshing](#), [Solving](#), and [Material Libraries](#).

ELECTRIC DISCHARGE INTERFACES

The [Electric Discharge Interfaces](#) chapter includes physics feature information and theory for physics interfaces under the Electric Discharge branch in the Model Wizard.

AC/DC INTERFACES

The [AC/DC Interfaces](#) chapter includes physics feature information and theory for physics interfaces under the AC/DC branch in the Model Wizard.

CHEMISTRY AND REACTION ENGINEERING INTERFACES

The [Chemistry and Reaction Engineering Interfaces](#) chapter includes physics feature information and theory for physics interfaces under the Chemical Species Transport branch in the Model Wizard.

RADIO FREQUENCY INTERFACES

The [Radio Frequency Interfaces](#) chapter includes physics feature information and theory for physics interfaces under the Radio Frequency branch in the Model Wizard.

Modeling Guidelines

In this chapter:

- [Connecting to Electrical Circuits](#)
- [SPICE Import and Export](#)
- [Meshing](#)
- [Solving](#)
- [Material Libraries](#)

Connecting to Electrical Circuits

In this section:

- [About Connecting Electrical Circuits to Physics Interfaces](#)
- [Connecting Electrical Circuits Using Predefined Couplings](#)
- [Connecting Electrical Circuits by User-Defined Couplings](#)
- [Solving](#)
- [Postprocessing](#)



Electrostatic Discharge: Application Library path
Electric_Discharge_Module/Electrostatic_Discharges/esd

About Connecting Electrical Circuits to Physics Interfaces

This section describes the various ways electrical circuits can be connected to other physics interfaces in COMSOL Multiphysics. If you are not familiar with circuit modeling, it is recommended that you review the [Theory for the Electrical Circuit Interface](#).

In general electrical circuits connect to other physics interfaces via one or more of three special circuit features:

- [External I vs. U](#)
- [External U vs. I](#)
- [External I-Terminal](#)

These features either accept a voltage measurement from the connecting noncircuit physics interface and return a current from an Electrical Circuit interface or the other way around.



The “External” features are considered “ideal” current or voltage sources by the Electrical Circuit interface. Hence, you cannot connect them directly in parallel (voltage sources) or in series (current sources) with other ideal sources. This results in the error message *The DAE is structurally inconsistent*. A workaround is to provide a suitable parallel or series resistor, which can be tuned to minimize its influence on the results.

Connecting Electrical Circuits Using Predefined Couplings

In addition to these circuit features, interfaces in the AC/DC Module, RF Module, MEMS Module, Electric Discharge Module, Plasma Module, and Semiconductor Module (the modules that include the Electrical Circuit interface) also contain features that provide couplings to the Electrical Circuit interface by accepting a voltage or a current from one of the specific circuit features ([External I vs. U](#), [External U vs. I](#), and [External I-Terminal](#)).

This coupling is typically activated when:

- A choice is made in the **Settings** window for the noncircuit physics interface feature, which then announces (that is, includes) the coupling to the Electrical Circuit interface. Its voltage is then included to make it visible to the connecting circuit feature.
- A voltage that has been announced (that is, included) is selected in a feature node’s **Settings** window.

These circuit connections are supported in Terminals.

Connecting Electrical Circuits by User-Defined Couplings

A more general way to connect a physics interface to the Electrical Circuit interface is to:

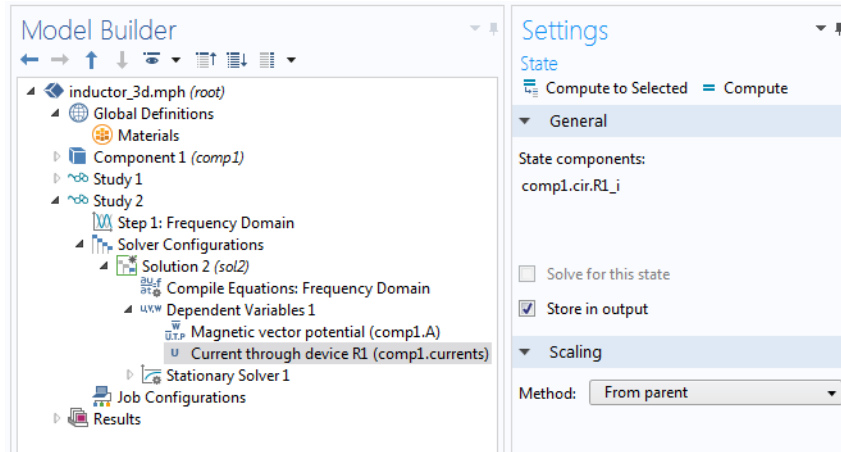
- Apply the voltage or current from the connecting “External” circuit feature as an excitation in the noncircuit physics interface.

- Define your own voltage or current measurement in the noncircuit physics interface using variables, coupling operators, and so forth.
- In the **Settings** window for the Electrical Circuit interface feature, selecting the User-defined option and entering the name of the variable or expression using coupling operators defined in the previous step.

DETERMINING A CURRENT OR VOLTAGE VARIABLE NAME

To determine a current or voltage variable name, look at the **Dependent Variables** node under the **Study** node. To do this:

- 1 In the **Model Builder**, right-click the **Study** node and select **Show Default Solver**.
- 2 Expand the **Solver > Dependent Variables** node and click the state node, in this example, **Current through device R1 (comp1.currents)**. The variable name is shown in the **Settings** window for **State**.



Typically, voltage variables are named `cir.Xn_v` and current variables `cir.Xn_i`, where n is the “External” device number — 1, 2, and so on.



Some modeling errors lead to the error message *The DAE is structurally inconsistent* being displayed when solving. This error typically occurs from having an open current loop, from connecting voltage sources in parallel, or connecting current sources in series.

In this respect, the predefined coupling features are also treated as (ideal) voltage or current sources. The remedy is to close current loops and to connect resistors in series with voltage sources or in parallel with current sources.

Postprocessing

The Electrical Circuits interface, unlike most of the other physics interfaces, solves for a relatively large number of global dependent variables (such as voltages and currents), instead of solving for a few space-varying fields (such as temperature or displacement). For this reason, the Electrical Circuit interface does not provide default plots when computing a study.

The physics interface defines a number of variables that can be used in postprocessing. All variables defined by the Electrical Circuit interface are of a global scope, and can be evaluated in a **Global Evaluation** node (under **Derived Values**). In addition, the time evolution or dependency on a parameter can be plotted in a **Global** plot (under a **ID Plot Group** node).

The physics interface defines a Node voltage variable for each electrical node in the circuit, with name `cir.v_name`, where `cir` is the physics interface Label and `<name>` is the node Name. For each two-pin component, the physics interface also defines variables containing the voltage across it and the current flowing through it. For resistors it adds a heat source variable as well.



In the *COMSOL Multiphysics Reference Manual*:

- [Derived Values, Evaluation Groups, and Tables and Global Evaluation](#)
 - [Plot Groups and Plots and Global](#)
-

SPICE Import and Export

SPICE Import

The circuit definition in COMSOL Multiphysics adheres to the SPICE format developed at the University of California, Berkeley (see [Ref. 1](#) for further information and references). SPICE netlists can be imported and the corresponding circuit nodes are generated in the COMSOL Multiphysics model. Most circuit simulators can export to this format or some version of it.

The Electrical Circuit interface supports the following device models:

TABLE 2-1: SUPPORTED SPICE DEVICE MODELS.

STATEMENT	DEVICE MODEL
R	Resistor
C	Capacitor
L	Inductor
V	Voltage Source
I	Current Source
E	Voltage-Controlled Voltage Source
F	Current-Controlled Current Source
G	Voltage-Controlled Current Source
H	Current-Controlled Voltage Source
D	Diode
Q	NPN BJT and PNP BJT
M	n-Channel MOSFET and p-Channel MOSFET
X	Subcircuit Instance

Statements corresponding to multiple devices are resolved by parsing the associated `.model` statement. The physics interface also supports the `.subckt` statement, which is represented in COMSOL by a [Subcircuit Definition](#) node, and the `.include` statement. SPICE commands are interpreted case-insensitively. The statement defining each device is also interpreted as the **Device name**.

According to SPICE specification, the first line in the netlist file is assumed to be the title of the netlist and it is ignored by the parser.

SPICE Export

The **SPICE Export** functionality creates a SPICE netlist file containing a description of the circuit represented by the physics interface. This functionality can be accessed from the physics interface context menu (right-click the physics interface node and select **Export SPICE Netlist**). After specifying a filename, the circuit is exported and messages from the export process display in the **Messages** window. During the export process, a series of operations are performed:

- In order to avoid conflicts, each component must be identified by a unique **Device name**. If one or more components have the same device name, the export operation fails and an error message is displayed. All characters in a **Device name** that are not letters, digits, or underscores are replaced by underscores.
- According to the SPICE specification, each circuit must have a node with name 0, which is assumed to be the only ground node. When exporting a circuit, any node with name 0 that is not connected to a **Ground** component is exported with a different node name. All nodes that are connected to a Ground components are exported as a merged node with name 0. The Messages window shows a log message if these operations are performed, showing the name of the renamed or merged nodes.
- All characters in node names that are not letters, digits, or underscores are replaced by underscores.
- Some components (most notably, the **External** components used to couple to other physics interfaces) cannot be exported to a SPICE netlist. These components are ignored during the export process, and a message is shown in the Messages window. Note that this can change the exported circuit, since some components are then missing.
- Subcircuit definitions are added as `.subckt` statements in the netlist. Semiconductor devices (such as MOSFETs, BJTs, and diodes) are exported as a SPICE device with a corresponding `.model` statement.

The title of the exported netlist file is the model's filename, and the time, date, and version of COMSOL Multiphysics is added as a comment in the netlist file.



Reference

1. <https://en.wikipedia.org/wiki/SPICE>

Meshing

The mesh is an important component of any numerical model of an electric discharge model. When assessing a numerical solution it is always important to ensure that the results do not change significantly when the mesh is refined; this is sometimes referred to as *mesh independence*. The Electric Discharge Module includes default mesh suggestions that automatically refine the mesh based on the physics features selected. In most cases manually tuning the default mesh improves performance and helps with the solution process.

Modeling different types of electric discharges typically requires varied strategies. Generally, regions like the streamer channel and corona discharge layer necessitate a finer mesh. Since electric discharge models solve transport equations, mapped and boundary layer meshes are often employed. It's also beneficial to use a coarser mesh in areas where discharges are weak to reduce the degrees of freedom (DoFs).

	For more details on setting up a meshing sequence, see the Meshing chapter in the <i>COMSOL Multiphysics Reference Manual</i> .
	<ul style="list-style-type: none">• <i>Positive Streamer Propagation in Transformer Oil</i>: Application Library path Electric_Discharge_Module/Liquid_Dielectrics/streamer_in_transformer_oil• <i>Negative Surface Discharge at Gas–Solid Interface</i>: Application Library path Electric_Discharge_Module/Dielectric_Barrier_Discharges/negative_surface_discharge

Solving

The dependent variables of the transport equations solved by the Electric Discharge interface are expressed in logarithmic form. The initial condition for the carrier number density cannot be zero and is set to a finite small value by default. For transient models, it is often necessary to add an Electrostatics Initialization study step before the Time Dependent study step such that the transient study has good and consistent initial values.

Note also that the solution from one study can be used as the starting point for a second study by altering the settings in the **Values of Dependent Variables** section of the **Stationary** study step. To do this, select the **Initial values of variables solved for** checkbox, select **Solution** for the **Method**, and then select the appropriate solution from the **Study** list.



In the *COMSOL Multiphysics Reference Manual*:

- [Introduction to Solvers and Studies](#)
- [Study and Study Step Types](#)
- [Computing a Solution](#)
- [Solution Operation Nodes and Solvers](#)

Material Libraries


The Electric Discharge Module features two Material Library datasets with materials properties to assist in modeling electric discharges.

The [Electric Discharge Material Library](#)¹ contains material property data for modeling charge transport in gases, liquids, and solids.

The [Equilibrium Discharge Material Library](#) contains material property data for modeling electric arc discharges with the magnetohydrodynamics model.

1. The material data of Transformer Oil is reproduced from J. Jadidian et. al, “Stochastic and deterministic causes of streamer branching in liquid dielectrics”, Journal of Applied Physics, vol. 114, no. 6, pp. 63301-1–10, 2013 (<https://doi.org/10.1063/1.4816091>), with the permission of AIP Publishing. The material data of Air [Morrow and Lowke, 1997] is reproduced from R. Morrow and J. J. Lowke, “Streamer propagation in air”, Journal of Physics D: Applied Physics, vol. 30, no. 4, pp. 614–627, 1997, with the permission of IOP Publishing. The material data of Polyethylene is reproduced from S. Le Roy et. al, “Description of charge transport in polyethylene using a fluid model with a constant mobility: fitting model and experiments”, Journal of Physics D: Applied Physics, vol. 39, no. 7, pp. 1427–1436, 2006, with the permission of IOP Publishing.



Electric Discharge Interfaces

This chapter describes the usage and theory for the physics interfaces found under the **Electric Discharge** branch ()

In this chapter:

- [The Electric Discharge Interface](#)
- [The Arc Discharge Multiphysics Interface](#)
- [The Transport of Charge Carriers Interface](#)
- [Theory for the Electric Discharge Interface](#)
- [Theory for the Arc Discharge Multiphysics Interface](#)
- [Theory for the Transport of Charge Carriers Interface](#)

The Electric Discharge Interface

The **Electric Discharge (edis)** interface (), found under the **Electric Discharge** branch (), is used to simulate electric discharges and predict electrical breakdown in gas, liquid, and solid dielectrics. It contains built-in charge transport models that solve the drift-diffusion equations of electrons, holes, as well as positive and negative ions fully coupled with Poisson's equation. In addition, it can also model the surface charge accumulation and relaxation effect at dielectric interfaces. Typical modeling applications are streamer discharges, corona discharges, electrostatic discharges, and dielectric barriers discharges. The effect of a background magnetic field or a flow field can be easily considered by coupling to another physics interface such as the *Magnetic Fields* or *Laminar Flow*.

The interface supports simulation of electric discharges in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. Stationary; time dependent; and frequency dependent, perturbation study types are available for the interface.



Theory for the Electric Discharge Interface

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the **name** string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is **edis**.

DOMAIN SELECTION

If any part of the model geometry should not partake in the transport model, remove that part from the selection list.

PHYSICAL MODEL

Dielectric Medium Selection

Use the checkboxes available to add dielectric medium to be modeled. See [Overview of Physical Models](#) for more details. There are three types of mechanisms that can be freely combined:

- **Gas**: which is selected by default for modeling gas discharges.
- **Liquid**: select this box when the system has liquid dielectric such as transformer oil.
- **Solid**: select this box when the system has solid dielectrics such as insulators, good and poor conductors, rubber, plastic, and so on.


Out-of-Plane Thickness

For 2D component and 1D axisymmetric components, the **Out-of-plane thickness** d_z (default value: 1 cm) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross section. Only constant thickness is supported. The value of this parameter is used, among other things, to automatically calculate the electric current flowing across the boundary.


CROSS-SECTIONAL AREA

For 1D components, enter a **Cross-sectional area** A_c to define a parameter for the area of the geometry perpendicular to the 1D component. Only constant thickness is supported. The value of this parameter is used, among other things, to automatically calculate the electric current flowing across the boundary. The default is 1 cm².

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button () and select **Stabilization**. By default, the **Streamline diffusion** checkbox is selected. The streamline diffusion stabilization does not change the original equation but adds the diffusion in the weak form and it vanishes once the original equation is converged. Use it when the transport equation is drift or convection-dominated. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.


INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button () and select **Stabilization**. By default, the **Isotropic diffusion** checkbox is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems. To add isotropic diffusion, select the **Isotropic diffusion** checkbox. The field for the **Tuning parameter** δ_{id} then becomes available. The default

value is 0.1; increase or decrease the value of δ_{id} to increase or decrease the amount of isotropic diffusion. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.

DISCRETIZATION

Use this section to change the discretization of the transport equations and Poisson's equation. Two formulations — **Finite element, log formulation (linear shape function)** (the default) and **Finite element, log formulation (quadratic shape function)** — are available for the discretization of *Charge carriers*. Three formulations — **Finite element (linear shape function)** (the default), **Finite element (quadratic shape function)**, and **Finite element (cubic shape function)** — are available for the discretization of *Electric potential*.

To display all settings available in this section, click the **Show More Options** button () and select **Advanced Physics Options**.

The **Compute boundary fluxes** checkbox is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variable affected in the interface is `ntflux_c` (where *c* is the carrier name). This is the normal total flux and corresponds to all flux contributions (drift, convection, and diffusion).

Also the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is selected. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see [Computing Accurate Fluxes](#) in the *COMSOL Multiphysics Reference Manual*.

The **Value types when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a

frequency-domain study. For more information, see [Splitting Complex-Valued Variables](#) in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variables are named as **Space charge density** rho and **Electric potential** V by default. The names must be unique with respect to all other dependent variables in the component.

Note that all physics features might add additional dependent variables depending on feature settings. For example, the **Gas** feature adds the natural logarithm of the number density of electrons, positive ions, and negative ions if the **Material model** is set to **Charge transport** and **Charge carriers** is set to **Electrons, positive and negative ions**. Note that these dependent variables added by physics features are not shown in this section.

You can access the number density of a carrier *c* (e, h, p, n for electrons, holes, positive ions, and negative ions, respectively) through the physics scope variable *name.n_c* where *name* is the physics interface name, as described earlier. Note that for **Finite element, log formulation**, the actual dependent variable is the natural logarithm of the number density divided by one per cubic centimeter, which is named as *name.logn_c* and defined as $\log(n_c/(1\text{ cm}^{-3}))$.

Domain, Boundary, and Pair Nodes for the Electric Discharge Interface

The Electric Discharge interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).



- To add a node, go to the **Physics** toolbar, no matter what operating system you are using.
- Contextual subnodes (attributes) are available by clicking the parent node in the Model Builder, and then selecting the subnode from the **Attributes** menu.

- Dielectric Interface, Bulk Transport
- Dielectric Interface, Surface Transport
- Electrode
- Gas
- Initial Values
- Insulation
- Liquid
- Photoionization
- Reactions
- Solid



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.



In the *COMSOL Multiphysics Reference Manual*, see [Table 2-4](#) for links to common sections and [Table 2-5](#) for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Gas

The **Gas** node defines the properties and the model formulation of a gas domain.



- [Gas Discharges](#)
- [Additional Transport Mechanisms](#)

MODEL INPUT

Gas properties, such as temperature and absolute pressure, can be defined through user inputs or variables, or by selecting a physics interface.

Temperature

By default, the **Temperature** model input is set to **User defined** and T can be manually prescribed. You can also select **Common model input**, and then the temperature is controlled from [Default Model Inputs](#) under **Global Definitions** or by a locally defined [Model Input](#). If a heat transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For

example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T .

Absolute Pressure

By default, the **Absolute pressure** model input is set to **User defined** and p_A can be manually prescribed. You can also select **Common model input**, and then the absolute pressure is controlled from **Default Model Inputs** under **Global Definitions** or by a locally defined **Model Input**. If a Fluid Flow interface is included in the component, it controls the absolute pressure **Common model input**. Alternatively, the absolute pressure field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Laminar Flow interface is included in the component, the **Absolute pressure (spf)** option is available for p_A .



Model Inputs and Multiphysics Couplings in the *COMSOL Multiphysics Reference Manual*

MODEL FORMULATION

In this section, select either **Insulator**, **Conductor**, or **Charge transport** from the **Material model** list. The **Insulator** option is equivalent to the Charge Conservation feature in the *Electrostatics* interface and it only adds Poisson's equation for the selected domain. The **Conductor** option is equivalent to the Current Conversation feature in the *Electric Currents* interface. The **Charge transport** option is used when you want to model and solve charge carriers explicitly.

Different charge transport models are supported. Choose one from the **Charge carriers** list. In the **Gas** domain, three options are available: **Electrons, positive and negative ions**; **Electrons and positive ions**; and **Positive and negative ions**.

CONSTITUTIVE RELATION D-E

Select a **Dielectric model** to describe the macroscopic properties of the medium (relating the electric displacement **D** with the electric field **E**) and the applicable material properties, such as the relative permittivity. Two options, **Relative permittivity** and **Polarization**, are available:

- **Relative permittivity** (the default) to use the constitutive relation $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$. Then the default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From**

material. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is 1.

- **Polarization** to use the constitutive relation $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$. Then enter the components based on space dimension for the **Polarization** vector \mathbf{P} (SI unit: C/m²). The defaults are 0 C/m².

CONSTITUTIVE RELATION JC-E

This section is shown only when the **Material model** is **Conductor**. By default, the **Electric conductivity** σ (SI unit: S/m) for the media is defined **From material**. Or select **User defined**:

User Defined

For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** depending on the characteristics of the electric conductivity, and then enter values or expressions for the electric conductivity σ in the field or matrix. The default is 1 S/m. You can also enter an expression for the conductivity as a function of temperature or other variables.

TRANSPORT PROPERTIES

This section is shown only when the **Material model** is **Charge transport**.

Transport Mechanisms

Use the checkboxes available to control transport mechanisms. There are four types of mechanisms that can be freely combined:

- **Electric field drift**, which is selected by default and considers the drift of charged species in an electric field. This checkbox cannot be cleared, which means that the drift of charged species in the electric field is always considered.
- **Magnetic field drift**, which considers the drift of charged species in a magnetic field.
- **Convection**, which models the background fluid flow where all species drift with the flow field.
- **Diffusion**, which models transport due to carrier density gradients.

Drift

By default, charge carrier mobility is set to **From material**. It will automatically pick up the material available in the **Materials** node in the **Model Builder**. Materials can be added from the **Electric Discharge** folder in the **Material Library**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is 1 m²/(V·s).

Diffusion

By default, the diffusion coefficient is computed from the mobility with the **Einstein relation**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is $10^{-5} \text{ m}^2/\text{s}$.

REACTIONS

Impact ionization

For **Charge transport** models including electrons, define the ionization coefficient **From material** or **User defined**.

Attachment

For **Charge transport** models including electrons and negative ions, define the attachment coefficient **From material** or **User defined**.

Recombination

Define the electron–ion recombination coefficient or ion–ion recombination coefficient **From material** or **User defined**.

Liquid

The **Liquid** node defines the properties and the model formulation of a liquid domain.



- [Discharges in Liquids](#)
- [Additional Transport Mechanisms](#)

MODEL INPUT

Liquid temperature can be defined through user inputs or variables, or by selecting a physics interface.

Temperature

By default, the **Temperature** model input is set to **User defined** and T can be manually prescribed. You can also select **Common model input**, and then the temperature is controlled from [Default Model Inputs](#) under **Global Definitions** or by a locally defined [Model Input](#). If a heat transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For

example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T .



MODEL FORMULATION

In this section, select either **Insulator**, **Conductor**, or **Charge transport** from the **Material model** list. The **Insulator** option is equivalent to the Charge Conservation feature in the *Electrostatics* interface and it only adds Poisson's equation for the selected domain. The **Conductor** option is equivalent to the Current Conversation feature in the *Electric Currents* interface. The **Charge transport** option is used when you want to model and solve charge carriers explicitly.

Different charge transport models are supported. Choose one from the **Charge carriers** list. In the **Liquid** domain, three options are available: **Electrons, positive and negative ions**; **Electrons and positive ions**; and **Positive and negative ions**.

CONSTITUTIVE RELATION D-E

Select a **Dielectric model** to describe the macroscopic properties of the medium (relating the electric displacement \mathbf{D} with the electric field \mathbf{E}) and the applicable material properties, such as the relative permittivity. Two options, **Relative permittivity** and **Polarization**, are available:

- **Relative permittivity** (the default) to use the constitutive relation $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$. Then the default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is 1.
- **Polarization** to use the constitutive relation $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$. Then enter the components based on space dimension for the **Polarization** vector \mathbf{P} (SI unit: C/m²). The defaults are 0 C/m².

CONSTITUTIVE RELATION J-C-E

This section is shown only when the **Material model** is **Conductor**. By default, the **Electric conductivity** σ (SI unit: S/m) for the media is defined **From material**. Or select **User defined**:

User Defined

For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** depending on the characteristics of the electric conductivity, and then enter values or expressions for the electric conductivity σ in the field or matrix. The default is 1 S/m. You can also enter an expression for the conductivity as a function of temperature or other variables.

TRANSPORT PROPERTIES

This section is shown only when the **Material model** is **Charge transport**.

Transport Mechanisms

Use the checkboxes available to control transport mechanisms. There are four types of mechanisms that can be freely combined:

- **Electric field drift**, which is selected by default and considers the drift of charged species in an electric field. This checkbox cannot be cleared, which means that the drift of charged species in the electric field is always considered.
- **Magnetic field drift**, which considers the drift of charged species in a magnetic field.
- **Convection**, which models the background fluid flow where all species drift with the flow field.
- **Diffusion**, which models transport due to carrier density gradients.

Drift

By default, charge carrier mobility is set to **From material**. It will automatically pick up the material available in the **Materials** node in the **Model Builder**. Materials can be added from the Electric Discharge folder in the **Material Library**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is $1 \text{ m}^2/(\text{V}\cdot\text{s})$.

Diffusion

By default, the diffusion coefficient is computed from the mobility with the **Einstein relation**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is $10^{-5} \text{ m}^2/\text{s}$.

REACTIONS

Field ionization

For **Charge transport** models including electrons, define the field ionization parameters **From material** or **User defined**.

Attachment

For **Charge transport** models including electrons and negative ions, define the attachment time constant **From material** or **User defined**.

Recombination

Define the electron–ion recombination coefficient or ion–ion recombination coefficient **From material** or **User defined**.

Solid

The **Solid** node defines the properties and the model formulation of a solid domain.



- [Bipolar Charge Transport in Solids](#)
- [Additional Transport Mechanisms](#)

MODEL INPUT

Solid temperature can be defined through user inputs or variables, or by selecting a physics interface.

Temperature

By default, the **Temperature** model input is set to **User defined** and T can be manually prescribed. You can also select **Common model input**, and then the temperature is controlled from [Default Model Inputs](#) under **Global Definitions** or by a locally defined [Model Input](#). If a heat transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T .



[Model Inputs and Multiphysics Couplings](#) in the *COMSOL Multiphysics Reference Manual*

MODEL FORMULATION

In this section, select either **Insulator**, **Conductor**, or **Charge transport** from the **Material model** list. The **Insulator** option is equivalent to the Charge Conservation feature in the *Electrostatics* interface and it only adds Poisson’s equation for the selected domain. The **Conductor** option is equivalent to the Current Conversation feature in the *Electric Currents* interface. The **Charge transport** option is used when you want to model and

solve charge carriers explicitly. The **Electrons and holes, mobile and trapped** model is available.

CONSTITUTIVE RELATION D-E

Select a **Dielectric model** to describe the macroscopic properties of the medium (relating the electric displacement **D** with the electric field **E**) and the applicable material properties, such as the relative permittivity. Two options, **Relative permittivity** and **Polarization**, are available:

- **Relative permittivity** (the default) to use the constitutive relation $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$. Then the default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is 1.
- **Polarization** to use the constitutive relation $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$. Then enter the components based on space dimension for the **Polarization** vector **P** (SI unit: C/m²). The defaults are 0 C/m².

CONSTITUTIVE RELATION JC-E

This section is shown only when the **Material model** is **Conductor**. By default, the **Electric conductivity** σ (SI unit: S/m) for the media is defined **From material**. Or select **User defined**:

User Defined

For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** depending on the characteristics of the electric conductivity, and then enter values or expressions for the electric conductivity σ in the field or matrix. The default is 1 S/m. You can also enter an expression for the conductivity as a function of temperature or other variables.

TRANSPORT PROPERTIES

This section is shown only when the **Material model** is **Charge transport**.

Transport Mechanisms

Use the checkboxes available to control transport mechanisms. There are four types of mechanisms that can be freely combined:

- **Electric field drift**, which is selected by default and considers the drift of charged species in an electric field. This checkbox cannot be cleared, which means that the drift of charged species in the electric field is always considered.
- **Magnetic field drift**, which considers the drift of charged species in a magnetic field.

- **Convection**, which is disabled for the **Solid** feature.
- **Diffusion**, which models transport due to carrier density gradients.

Drift

The electron and hole mobility is computed from the band mobility and the depth of shallow traps. By default, electron and hole band mobilities are set to **From material**.

Diffusion

By default, the diffusion coefficient is computed from the mobility with the **Einstein relation**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is $10^{-5} \text{ m}^2/\text{s}$.

REACTIONS

This section is only shown when the **Charge transport** model is selected.

Detrapping

It contains several parameters to specify material data for detrapping effect.

Trapping

It contains several parameters to specify material data for trapping effect.

Recombination

It contains several parameters to specify material data for recombination effect.

Initial Values

The **Initial Values** node is a subfeature and it adds an initial value for the electric potential V and charge carrier density that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Electric potential** V (SI unit: V). The default value is 0 V. Depending on the **Material model** setting of its parent feature, enter a value or expression for the initial values of charge carrier densities.

Insulation

The **Insulation** node is a subfeature and it is added by default to all exterior boundaries of the selected domain for its parent feature. It is used to model electrically insulating boundaries that have no electric charge.

Dielectric Interface, Bulk Transport

The **Dielectric Interface, Bulk Transport** node is a subfeature and it is added by default to interface boundaries between different domains (**Gas**, **Liquid**, and **Solid**). It is used to specify boundary conditions for charge carriers. See [Charge Transport at Dielectric Interfaces](#) for more details.

Electrode

The **Electrode** node is a subfeature for modeling what happens when a dielectric is in contact with a metal surface.

	Electrode Boundary Condition
---	--

TERMINAL

Specify the terminal properties. To indicate which boundaries belong to the same terminal, enter the same name in the **Terminal** field.

Select a Terminal type — **Voltage** (the default) or **Circuit**:

- **Voltage** to enter an electric potential.
- **Circuit** to specify a terminal connected to an external circuit. The **Terminal** node provides a current-voltage characteristic to the circuit element.

CHARGE TRANSPORT

This section is available only when the **Material model** of its parent feature is **Charge transport**. It is used to specify boundary conditions for charge carriers at the metal surface. Available boundary conditions are **No diffusive flux** (the default), **Number density**, **Open boundary**, **No flux**, **Flux**, and **Surface emission** (for electrons and holes).

	General Charge Carrier Boundary Conditions
---	--

SURFACE EMISSION

This section is available only when the boundary condition of electrons or holes is set to **Surface emission**. Depending on the parent feature, different surface emission mechanisms are available.



Surface Emission

- **Secondary electron emission**: available when the parent feature is **Gas**.
- **Field electron emission**: available when the parent feature is **Gas**.
- **Thermionic emission**: available for all parent features.
- **Schottky effect (for thermionic emission)**: available when the parent feature is **Liquid** or **Solid**.

Generally, carriers drift inward to the boundary conditions. For outward-drifting carriers, two options, **Open boundary** and **No flux**, are available.

Dielectric Interface, Surface Transport

The **Dielectric Interface, Surface Transport** node is a default boundary feature for modeling surface charge dynamics at dielectric interfaces. The node is available when more than one dielectric medium in the **Physical Model** section is selected. It is always used together with the [Dielectric Interface, Bulk Transport](#) feature. See [Charge Transport at Dielectric Interfaces](#) for more details.

Reactions

Use the **Reactions** node to account for the consumption or production of species through additional reactions. This node is usually unnecessary, as the most important discharge chemistry is already added by the built-in charge transport model. Define the rate expressions as required.

REACTION RATES

Add a rate expression R_n for species n . Enter a value or expression in the field.

Photoionization

The **Photoionization** node is used to model photoionization, which is critical in positive gas discharges at both atmospheric and high pressure.





Photoionization

PHOTOIONIZATION

Select **Number of exponential terms**, **Element order** and define other parameters required by the photoionization model. The default is using three terms and linear element to model photoionization in air. The new electrons and positive ions generated by photoionization are added by the feature.

The Arc Discharge Multiphysics Interface

The **Arc Discharges** () multiphysics interface is used to study electric arc discharges (fully ionized) in a magnetohydrodynamics (MHD) framework. This multiphysics interface adds three single physics interfaces: Magnetic and Electric Fields, Heat Transfer in Fluids, and Laminar Flow, together with several multiphysics coupling features. The multiphysics couplings add the MHD coupling between the Magnetic and Electric Fields and the Laminar Flow interfaces. The multiphysics couplings also add heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating and radiation loss.

When a predefined **Arc Discharges** interface is added from the **Electric Discharge** branch () of the **Model Wizard** or **Add Physics** windows, **Magnetic and Electric Fields**, **Heat Transfer in Fluids**, and **Laminar Flow** interfaces are added to the Model Builder. In addition, the **Multiphysics Couplings** node is added, which automatically includes the multiphysics coupling features **Equilibrium Discharge Heat Source** and **Magnetohydrodynamics**.

On the Constituent Physics Interfaces

The Electric Discharge Module includes the essential features of its constituent physics interfaces. However, access to some advanced features and functionalities requires additional licenses, such as the AC/DC Module license or the CFD Module license.

The Magnetic and Electric Fields interface is used to compute magnetic field and induced current distributions in and around coils, conductors, and magnets. The Magnetic and Electric Fields interface solves Maxwell's equations formulated using the magnetic vector potential and, optionally for coils, the scalar electric potential as the dependent variables.

The Heat Transfer in Fluids interface provides features for modeling heat transfer by conduction, convection, and radiation. A Fluid model is active by default on all domains. All functionality for including other domain types, such as a solid domain, is also available. The temperature equation defined in solid domains corresponds to the differential form of the Fourier's law that may contain additional contributions like heat sources.

The Laminar Flow interface solves for conservation of energy, mass, and momentum in fluids.



For details about predefined multiphysics couplings, see [Multiphysics Modeling Workflow](#) in the *COMSOL Multiphysics Reference Manual*.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Arc Discharges**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Magnetic and Electric Fields**, **Heat Transfer in Fluids**, and **Laminar Flow** interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics Couplings** node. You can then choose from the available coupling features, **Equilibrium Discharge Heat Source**, **Magnetohydrodynamics**, **Nonisothermal Flow**, and **Equilibrium Discharge Boundary Heat Source** but the modified settings are not included.



Coupling features are available from the context menu (right-click the **Multiphysics Couplings** node) or from the **Physics** toolbar’s **Multiphysics** menu.

TABLE 3-1: MODIFIED SETTINGS FOR AN ARC DISCHARGE INTERFACE.

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Magnetic and Electric Fields	The discretization of the dependent variables is set to linear. The Ampère's Law and Current Conservation in Fluids feature is added.
Heat Transfer in Fluids	In the Fluid default feature, the Absolute pressure , p_A (Model Input section) and the Velocity field , \mathbf{u} (Heat Convection section) are set to Common model input .
Laminar Flow	The Compressibility option is set to Compressible flow (Ma<0.3) .

TABLE 3-1: MODIFIED SETTINGS FOR AN ARC DISCHARGE INTERFACE.

PHYSICS INTERFACE OR COUPLING FEATURE	MODIFIED SETTINGS
Equilibrium Discharge Heat Source	The Domain Selection is the same as that of the participating physics interfaces. The corresponding Magnetic Fields and Heat Transfer in Fluids interfaces are preselected in the Coupled Interfaces section.
Magnetohydrodynamics	The Domain Selection is the same as that of the participating physics interfaces. The corresponding Magnetic Fields and Laminar Flow interfaces are preselected in the Coupled Interfaces section.

PHYSICS INTERFACE AND COUPLING FEATURES



Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Coupling Features

- The [Equilibrium Discharge Heat Source](#) and [Equilibrium Discharge Boundary Heat Source](#) multiphysics coupling nodes are described in this chapter.
- The Magnetohydrodynamics multiphysics coupling node is described in this chapter.
- The [Nonisothermal Flow](#) coupling node is described for [The Nonisothermal Flow and Conjugate Heat Transfer Interfaces](#) in the *COMSOL Multiphysics Reference Manual*.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).




In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

- The available physics features for [The Laminar Flow Interface](#) are listed in the section [Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow](#).

- The available physics features for the heat transfer interfaces are listed in the sections [Domain Features](#), [Boundary Features](#), and [Edge and Point Features](#) in the *COMSOL Multiphysics Reference Manual*.
- The available physics features for [The Magnetic and Electric Fields Interface](#) are listed in the section [Domain, Boundary, Edge, Point, and Pair Nodes for the Magnetic and Electric Fields Interface](#).

Equilibrium Discharge Heat Source

The **Equilibrium Discharge Heat Source** multiphysics coupling () represents the source term Q (SI units: W/m^3) in the heat equation implemented by

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = Q \quad (3-1)$$

The source term Q includes three selectable source/sink components:

- Resistive heating (ohmic heating).

$$Q = \mathbf{J} \cdot \mathbf{E} \quad (3-2)$$

- Volumetric net radiation loss Q_{rad} defined by the total volumetric emission coefficient, which comes from a material property.
- Enthalpy transport (energy carried by the electric current)

$$\frac{\partial}{\partial T} \left(\frac{5k_B T}{2q} \right) (\nabla T \cdot \mathbf{J}) \quad (3-3)$$

Note that the enthalpy transport term prevails, for instance, in the boundary layers close to electrodes in a fully ionized electric discharge.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is `phs1`.

HEAT SOURCE COMPONENTS

By default, the **Include enthalpy transport**, **Include Joule heating**, and **Include volumetric net radiation loss** checkboxes are selected. From the list, select a **Total volumetric emission coefficient** Q_{rad} (SI unit: W/m^3) — **From material** (the default) or **User defined**. For **User defined**, enter a value or expression in the field. The heat source component are selectable in order to be able to see the effect of each of the component on the electric arc dynamics.

EQUILIBRIUM DISCHARGE HEAT SOURCE


This section defines the physics involved in the Equilibrium Discharge Heat Source multiphysics coupling. By default, the applicable physics interface is selected in the **Electromagnetic** list to apply the **Heat transfer** to its physics interface to establish the coupling.

You can also select **None** from either list to uncouple the **Equilibrium Discharge Heat Source** node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in Fluids** is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.



If a physics interface is deleted and then added to the model again, and in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See [Multiphysics Modeling Workflow](#) in the *COMSOL Multiphysics Reference Manual*.

Equilibrium Discharge Boundary Heat Source

The **Equilibrium Discharge Boundary Heat Source** multiphysics coupling () maps the electromagnetic surface losses as a heat source on the boundary (SI unit: W/m^2) in the heat transfer part of the model.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different coupling nodes or physics

interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is **bphs1**.

ELECTRODE PROPERTIES

Select an **Electrode polarity** — **Anode** (the default) or **Cathode**. Enter a **Surface work function** Φ (SI unit: V). The default is 4.15 V.

ELECTRON CURRENT


This section is available when **Cathode** is selected as the **Electrode polarity**.

Enter an **Effective Richardson's constant** A^*_R (SI unit: $\text{A}/(\text{m}^2 \cdot \text{K}^2)$). The default is $120 \text{ A}/(\text{m}^2 \cdot \text{K}^2)$. Enter an **Effective work function** Φ_{eff} (SI unit: V). The default is 2.6 V.

ION CURRENT

This section is available when **Cathode** is selected as the **Electrode polarity**. Enter a value or expression for the **Plasma's ionization potential** V_{ion} (SI unit: V). The default is 15.7 V.

SOURCE POSITION


To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

Select a **Source position** — **Layer** (the default), **Upside**, or **Downside**.

EQUILIBRIUM DISCHARGE BOUNDARY HEAT SOURCE

This section has the same setting information as defined under [Equilibrium Discharge Heat Source](#).

Magnetohydrodynamics

The **Magnetohydrodynamics** () multiphysics coupling feature is used to model the interaction of magnetic fields and conducting fluids. It couples one of the magnetic field interfaces and the **Laminar Flow** interface. The supported magnetic field interfaces are the **Magnetic Fields**, **Magnetic and Electric Fields**, **Magnetic Field Formulation**, and **Rotating Machinery**, **Magnetic** interfaces in the AC/DC Module. By default, the coupling feature passes the Lorentz force $\mathbf{F} = \mathbf{J} \times \mathbf{B}$ from the magnetic field interface to the **Laminar Flow** interface and the electromotive force (the induced electric field) $\mathbf{E} = \mathbf{v} \times \mathbf{B}$ from the **Laminar Flow** interface to the magnetic field interface.

The **Magnetohydrodynamics** feature is available in 2D, 2D axisymmetric, and 3D geometries and is allowed for both Stationary and Time Dependent studies (including Frequency-Stationary and Frequency-Transient studies). When the deformation of the conducting fluids cannot be neglected (that is, when topology changes are important), the **Moving Mesh** feature (added from the **Definitions**) is usually used together with the **Magnetohydrodynamics** feature.



- The **Magnetohydrodynamics** feature cannot be used to model magnetizable fluids (ferrohydrodynamics). In magnetizable fluids, the magnetization forces can be much larger than the Lorentz force. In such cases, a user-defined multiphysics coupling is required.
- The difference between the **Magnetic and Electric Fields** interface and the **Magnetic Fields** interface is that the former solves the current conservation equation explicitly, while the latter assumes the conservation of current implicitly. In 3D magnetohydrodynamics modeling, the most general approach is to use the **Magnetic and Electric Fields** interface to solve the magnetic field. The **Magnetic Fields**, **Magnetic Field Formulation**, and **Rotating Machinery**, **Magnetic** interfaces can be useful in specific cases.

SETTINGS

The **Label** is the multiphysics coupling feature name. The default **Label** (for the first multiphysics coupling feature in the model) is **Magnetohydrodynamics 1**.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the **name** string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature in the model) is **mhd1**.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Electromagnetic** and **Fluid flow** lists include all applicable physics interfaces.

When the Magnetohydrodynamics node is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (macOS and Linux users), or context menu (all

users), then the first physics interface of each type in the component is selected as the default.

You can also select **None** from either list to uncouple the Magnetohydrodynamics node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Solid Mechanics** is deleted, then the list defaults to **None** as there is nothing to couple to.





If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See [Multiphysics Modeling Workflow](#) in the *COMSOL Multiphysics Reference Manual*.

COUPLED SETTINGS

The coupling behavior can be easily controlled by selecting or clearing the **Include Lorentz force** and **Include electromotive force** checkboxes. For example, if **Include Lorentz force** is selected and **Include electromotive force** is cleared, only the Lorentz force is considered and the electromotive force is neglected. This is usually valid when the magnetic Reynolds number is very low.

The Transport of Charge Carriers Interface

The **Transport of Charge Carriers (tcc)** interface () , found under the **Electric Discharge** branch () , 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.

The interface supports simulation of charge transport in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. Stationary; time dependent; and frequency dependent, perturbation study types are available for the interface.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `tcc`.

DOMAIN SELECTION

If any part of the model geometry should not partake in the transport model, remove that part from the selection list.

OUT-OF-PLANE THICKNESS

For 2D component and 1D axisymmetric components, the **Out-of-plane thickness** d_z (default value: 1 cm) defines a parameter for the thickness of the geometry perpendicular to the two-dimensional cross section. Only constant thickness is supported. The value of this parameter is used, among other things, to automatically calculate the electric current flowing across the boundary.

CROSS-SECTIONAL AREA


For 1D components, enter a **Cross-sectional area** A_c to define a parameter for the area of the geometry perpendicular to the 1D component. Only constant area is supported. The value of this parameter is used, among other things, to automatically calculate the electric current flowing across the boundary. The default is 1 cm^2 .

TRANSPORT MECHANISMS


Use the checkboxes available to control transport mechanisms. There are four types of mechanisms that can be freely combined:

- **Electric field drift**, which is selected by default and it considers the drift of charged species in an electric field.
- **Magnetic field drift**, which considers the drift of charged species in a magnetic field.
- **Convection**, which models the background fluid flow where all species drift with the flow field.
- **Diffusion**, which is selected by default.

CONSISTENT STABILIZATION


To display this section, click the **Show More Options** button () and select **Stabilization**. By default, the **Streamline diffusion** checkbox is selected. The streamline diffusion stabilization does not change the original equation but adds the diffusion in the weak form and it vanishes once the original equation is converged. Use it when the transport equation is drift or convection-dominated. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.

INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button () and select **Stabilization**. By default, the **Isotropic diffusion** checkbox is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems. To add isotropic diffusion, select the **Isotropic diffusion** checkbox. The field for the **Tuning parameter** δ_{id} then becomes available. The default value is 0.1; increase or decrease the value of δ_{id} to increase or decrease the amount of isotropic diffusion. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.

DISCRETIZATION

Use this section to change the discretization of the transport equations. Two formulations, **Finite element**, **log formulation (linear shape function)** (the default) and **Finite element, log formulation (quadratic shape function)**, are available.

To display all settings available in this section, click the **Show More Options** button () and select **Advanced Physics Options**.

The **Compute boundary fluxes** checkbox is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the checkbox is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variable affected in the interface is `ntflux_c` (where *c* is the carrier name). This is the normal total flux and corresponds to all flux contributions (drift, convection, and diffusion).



Also the **Apply smoothing to boundary fluxes** checkbox is available if the previous checkbox is selected. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see [Computing Accurate Fluxes](#) in the *COMSOL Multiphysics Reference Manual*.

The **Value type when using splitting of complex variables** setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see [Splitting Complex-Valued Variables](#) in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variables are named as **Charge carriers *n*** by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove charge carriers in the model and also change the names accordingly. Enter the **Number of charge carriers**. Use the **Add Charge Carrier** () and **Remove Charge Carrier** () buttons as needed.

You can access the number density of a carrier c either as n_c or through the physics scope variable $name.n_c$ where $name$ is the physics interface name, as described earlier. Note that for **Finite element, log formulation**, the actual dependent variable is the natural logarithm of the number density divided by one per cubic centimeter, which is named as $name.logn_c$ and defined as $\log(n_c/(1\text{ cm}^{-3}))$.

Domain, Boundary, and Pair Nodes for the Transport of Charge Carriers Interface

The Transport of Charge Carriers interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).



- To add a node, go to the **Physics** toolbar, no matter what operating system you are using.
- Contextual subnodes (attributes) are available by clicking the parent node in the Model Builder, and then selecting the subnode from the **Attributes** menu.

- | | |
|--|---------------------------------------|
| • Transport Properties | • No Flux |
| • No Diffusive Flux | • Flux |
| • Initial Values | • Symmetry |
| • Reactions | • Periodic Condition |
| • Number Density | • Current Calculation |
| • Open Boundary | |



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.



In the *COMSOL Multiphysics Reference Manual*, see [Table 2-4](#) for links to common sections and [Table 2-5](#) for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Transport Properties

The settings in this node are dependent on the checkboxes selected under **Transport Mechanisms** in the **Settings** window for the Transport of Charge Carriers interface. It includes only the sections required by the activated transport mechanisms.

ELECTRIC FIELD

This section is available when the **Electric field drift** checkbox is selected. From the **Electric field** list, select the source of the electric field.

- Enter a value or expression for the **Electric field \mathbf{E}** , which is **User defined**; this input option is always available.
- Select the electric field solved by another physics interface such as an **Electrostatics** or **Electric Discharge** interface that has also been added to the model.
- Or select the option **Common model input**.

MAGNETIC FIELD

This section is available when the **Magnetic field drift** checkbox is selected. From the **Magnetic flux density** list, select the source of the magnetic flux density.

- Enter a value or expression for the **Magnetic flux density \mathbf{B}** , which is **User defined**; this input option is always available.
- Select the magnetic field solved by another physics interface such as a **Magnetic Fields** interface that has also been added to the model.
- Or select the option **Common model input**.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**.

- For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

- You can also select the velocity field solved by another interface such as **Laminar Flow** interface that has also been added to the model.
- Or select the option **Common model input**.

DRIFT

This section is available when at least one of the **Electric field drift** and **Magnetic field drift** checkboxes is selected. Enter the **Charge number** z_n (dimensionless, but requires a plus or minus sign) for each charge carrier. For **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value of expression of the mobility μ_n .

DIFFUSION

This section is available when the **Diffusion** checkbox is selected. Use this section to specify diffusion coefficients describing the diffusion of each charge carrier in the solvent fluid.

Enter a value or expression for the **Diffusion coefficient** D_n of each charge carrier in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — that describes the diffusion transport, and then enter the values in the corresponding element (one value for each charge carrier).

No Diffusive Flux

This node is the default boundary condition on exterior boundaries and prescribes a vanishing flux due to diffusion across the boundary:

$$-\mathbf{n} \cdot (-D\nabla n) = 0$$

Initial Values

The **Initial Values** node specifies the initial values for the number density of each charge carrier. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression for the initial value of the number density, n_i . This also serves as a starting guess for stationary problems.

Reactions

Use the **Reactions** node to account for the consumption or production of charge carriers through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define a rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the model geometry.

REACTION RATES

Add a rate expression R_n for charge carrier n . Enter a value or expression in the field.

Number Density

This condition node adds a boundary condition for the charge carrier number density. For example, a $n = n_0$ condition specifies the number density of carrier n .


NUMBER DENSITY

Individually specify the number density for each charge carrier. Select the checkbox for the **Carrier** to specify the number density, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific carrier, click to clear the checkbox for the number density of that carrier.

BOUNDARY CONDITION FOR CARRIERS NOT SPECIFIED

Specify boundary conditions other than **Number Density** for charge carriers that were unchecked above. Choose from the list: **No diffusive flux**, **Open boundary**, or **No flux**.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options**. You can find details about the different constraint settings in the section [Constraint Reaction Terms](#) in the *COMSOL Multiphysics Reference Manual*

Open Boundary

Use this node to allow charge carriers to drift out of the domain, but by default, not allow inward flux.

No Flux

The **No Flux** boundary condition prescribes a zero total flux (insulation) across the boundary.

Flux

This node can be used to specify the charge carriers flux across a boundary. The flux can, for example, occur due to chemical reactions or a phase change at the boundary.

INWARD FLUX

Individually specify the flux for each charge carrier. Select the checkbox for the **Carrier** to specify the inward flux, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific carrier, click to clear the checkbox for the inward flux of that carrier.

BOUNDARY CONDITION FOR CARRIERS NOT SPECIFIED

Specify boundary conditions other than **Flux** for charge carriers that were unchecked above. Choose from the list: **No diffusive flux**, **Open boundary**, or **No flux**.

Symmetry

The **Symmetry** node can be used to represent boundaries where the charge carrier concentration is symmetric; that is, where there is no flux across the boundary.

This boundary condition is identical to that of the [No Diffusive Flux](#) node.

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the number density and the diffusive flux between the “source” and the “destination” side, respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.


BOUNDARY SELECTION

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.


DESTINATION SELECTION

For more complex geometries, it might be necessary to specify the destination selection manually. To do so, right-click the **Periodic Condition** node and choose **Manual Destination Selection**. You can then specify the boundaries that constitute the destination surfaces in the **Destination Selection** section.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog. This section contains settings for specifying the type of constraint and whether to use a pointwise or weak constraint. See [Constraint Settings](#) in the *COMSOL Multiphysics Reference Manual* for more information.


ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see [Orientation of Source and Destination](#) in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see [Orientation of Source and Destination](#) in the *COMSOL Multiphysics Reference Manual*.

MAPPING BETWEEN SOURCE AND DESTINATION

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Mapping Between Source and Destination** section, see [Mapping Between Source and Destination](#) in the *COMSOL Multiphysics Reference Manual*.

FURTHER READING

For an example of using a periodic condition, see this application example:



The KdV Equation and Solitons: Application Library path
COMSOL_Multiphysics/Equation_Based/kdv_equation

Current Calculation

Use this node to calculate the current passing the terminal that you specify under **Terminal name**. The total current is calculated by integrating the current density of charge carriers through the selected boundary S :

$$I_c = - \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{J}_c dS$$

where \mathbf{n} denotes the outward normal from the boundary.

Theory for the Electric Discharge Interface

The [The Electric Discharge Interface](#) can be used to model electrical discharges in gases (air, SF₆, CO₂, etc.), liquids (transformer oil, water, etc.), and solids (polyethylene, rubber, etc.), as well as the charge accumulation and relaxation effects at their interfaces. Typical modeling examples are streamer discharges, corona discharges, DBD, partial discharges, etc. This interface contains predefined discharge models that are ready to use.

In this section:

- [Review of Charge Relaxation](#)
- [Overview of Physical Models](#)
- [Gas Discharges](#)
- [Discharges in Liquids](#)
- [Bipolar Charge Transport in Solids](#)
- [Electrode Boundary Condition](#)
- [Charge Transport at Dielectric Interfaces](#)
- [Additional Transport Mechanisms](#)
- [Numerical Stabilization Technique](#)
- [References](#)

Review of Charge Relaxation

Starting from the [Charge Relaxation Theory](#), it is crucial to consider two distinct time scales when modeling charge dynamics. These time scales are:

- 1 The intrinsic *charge relaxation time* τ , which is a characteristic time scale for the redistribution of charges within a material.
- 2 The *external time scale* t , which corresponds to the duration over which a device is energized or the observation period.

By comparing these two time scales, we can define the behavior of materials as follows:

- **Insulator:** if $\tau \gg t$, charges do not have sufficient time to redistribute significantly. This scenario is typically modeled using the Electrostatics interface, where Poisson's equation is solved.
- **Conductor:** $\tau \ll t$, charges have ample time to redistribute. This is usually modeled using the Electric Currents interface, which solves the current conservation equation.

In more complex cases where charge dynamics cannot be easily prescribed, a separate charge transport formulation is required. Various specialized modules are available for different types of problems:

- The **Plasma Module** focuses on modeling low-pressure plasma reactors in gases.
- The **Electrochemistry Module** is designed for modeling interactions between chemical and electrical energy in liquid electrolytes.
- The **Semiconductor Module** is primarily used for modeling crystalline solids based on band-gap theory.
- The **Electric Discharge Module** addresses modeling electric discharges and breakdowns in gases, liquids, and solids.

These add-on products offer tailored solutions for specific charge transport challenges across different environments.

Overview of Physical Models

The Electric Discharge interface supports three types of dielectric media: gas, liquid, and solid. Within each dielectric domain, three material models can be applied: insulator, conductor, and charge transport. The specific transport equations vary depending on the type of medium being modeled.

As shown in [Figure 3-1](#), a typical model consists of three domains. These domains represent the regions where charge transport and discharge phenomena occur, each characterized by specific material properties. Boundary features define the interactions at the edges of these domains, including insulating boundaries, electrodes, and interfaces between different media.

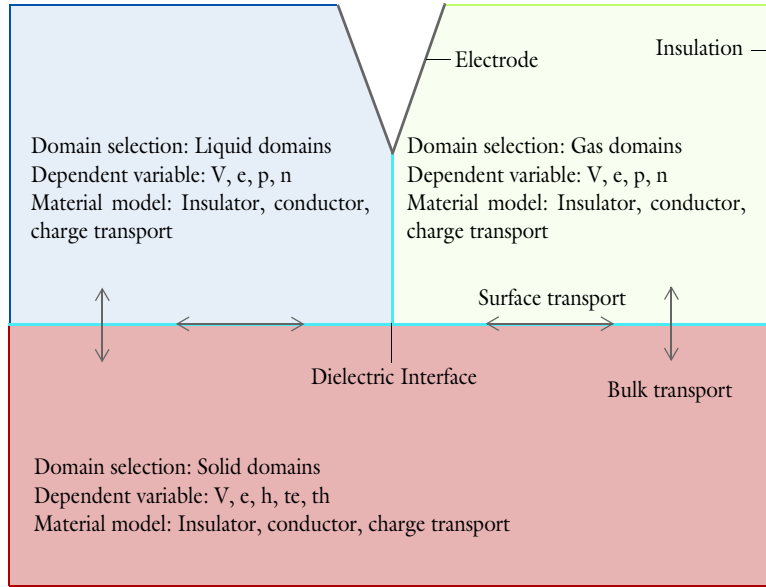


Figure 3-1: A general model considered by the Electric Discharge interface. The symbols e , h , p , n , te , th are short for electrons, holes, positive ions, negative ions, trapped electrons, and trapped holes.

Electric discharges are primarily driven by the electric field \mathbf{E} . In the Electric Discharge interface, the electric potential V is introduced to solve for \mathbf{E} :

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

where V is a dependent variable that is solved across all domains. By default, the constitutive relation between the electric field \mathbf{E} and the displacement field \mathbf{D} is:

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

where ϵ_0 (SI unit: F/m) is the permittivity of vacuum, ϵ_r is the relative permittivity. Alternative dielectric models, such as those incorporating polarization effects, are also available.

INSULATOR

For **Insulator** material model, Poisson's equation is solved. The equation is the same for both stationary and time-dependent studies:

$$\nabla \cdot \mathbf{D} = \rho$$

where ρ (SI unit: C/m³) is the space charge density.

CONDUCTOR

For **Conductor** material model, the current conservation equation is solved:

$$\begin{aligned}\nabla \cdot (\mathbf{J}_c + \mathbf{J}_d) &= 0 \\ \mathbf{J}_c &= \sigma \mathbf{E} \\ \mathbf{J}_d &= \frac{\partial \mathbf{D}}{\partial t}\end{aligned}$$

where \mathbf{J}_c and \mathbf{J}_d represent the conduction and displacement current densities, respectively.

CHARGE TRANSPORT FORMULATION

In general, the charge transport model solves for electrons (e), positive ions (p), and negative ions (n) in gas and liquid domains, while in solid domains, it solves for electrons (e), holes (h), and trapped electrons and holes (te, th).

Next, we will delve deeper into the theory of electric charge transport models in gases, liquids, and solids.

Gas Discharges

FLUID APPROXIMATION

The Electric Discharge interface, like the Plasma interface, relies on the fluid approximation, which uses a single-moment description based on continuity equations. This approximation is generally valid when the product of gas pressure p and discharge gap length d exceeds 0.1 Torr-cm. If $p \cdot d$ falls below 0.1 Torr-cm, the fluid model becomes inaccurate, and particle models are required. For instance, with a discharge gap of 1 cm, the lowest pressure that can be accurately modeled is approximately 0.1 Torr (13.332 Pa). The fluid approximation remains valid for reduced electric fields up to 1500 Td ([Ref. 1](#)).

LOCAL FIELD APPROXIMATION

The behavior of electric discharges differs significantly under varying pressure-gap products $p \cdot d$. For atmospheric pressure discharges, where $p \cdot d$ exceeds 200 Torr-cm,

the Local Field Approximation (LFA) is commonly applied. The Electric Discharge interface is particularly focused on modeling such conditions, as shown in [Figure 3-2](#).

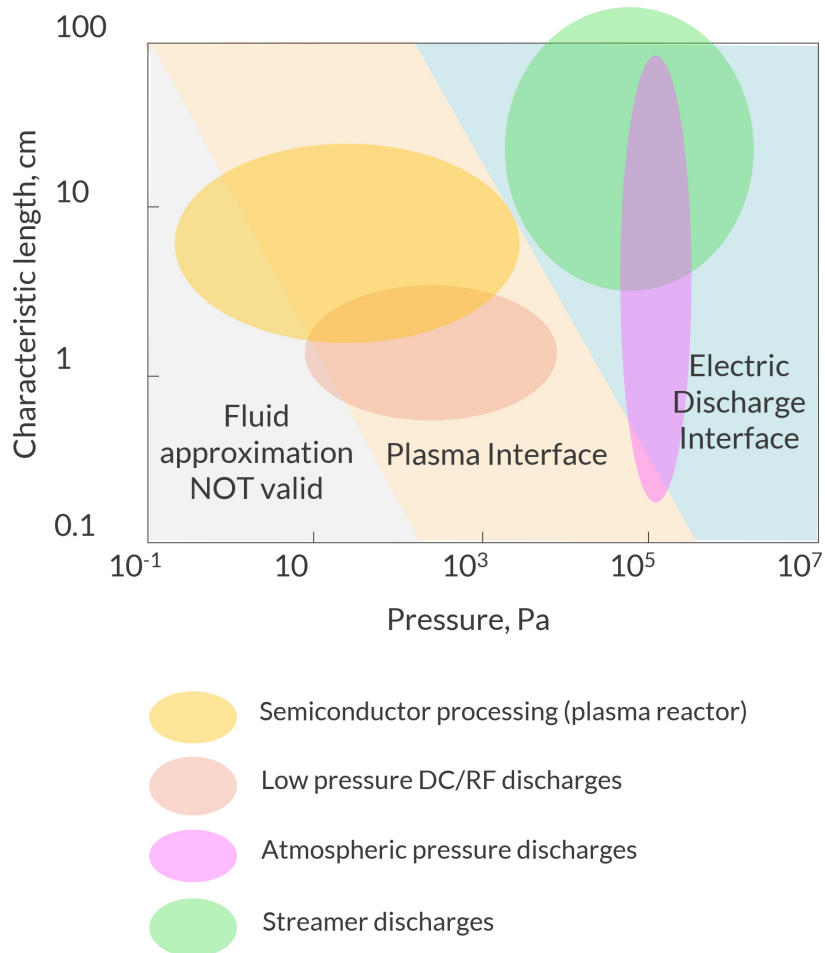


Figure 3-2: General guidelines for choosing the Plasma interface or the Electric Discharge interface when modeling gas discharges.

GOVERNING EQUATIONS

The Electric Discharge interface provides built-in charge transport models in gases. The default model consists of a group of transport equations for each modeled charge carrier ([Ref. 1](#)):

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{w}_i n_i - D_i \nabla n_i) = R_i$$

where

$$i = e, p, n$$

$$z_{e, p, n} = -1, +1, -1$$

$$\mathbf{w}_i = z_i \mu_i \mathbf{E}$$

$$R_e = \alpha |\mathbf{w}_e| n_e - \eta |\mathbf{w}_e| n_e - \beta_{ep} n_e n_p$$

$$R_p = \alpha |\mathbf{w}_e| n_e - \beta_{ep} n_e n_p - \beta_{pn} n_p n_n$$

$$R_n = \eta |\mathbf{w}_e| n_e - \beta_{pn} n_p n_n$$

where

- e, p, n denote electrons, positive ions, and negative ions
- n_i is the number density of the charge carrier (SI unit: $1/\text{m}^3$)
- \mathbf{E} is the electric field (SI unit: V/m)
- z_i denotes the carrier charge (SI unit: 1)
- μ_i denotes the carrier mobility (SI unit: $\text{m}^2/(\text{V}\cdot\text{s})$)
- \mathbf{w}_i is the drift velocity in the electric field (SI unit: m/s)
- D_i is the diffusion coefficient (SI unit: m^2/s)
- R_i is the reaction rate (SI unit: $1/(\text{m}^3\cdot\text{s})$)
- α is the ionization coefficient (SI unit: $1/\text{m}$)
- η is the attachment coefficient (SI unit: $1/\text{m}$)
- β_{ep} is the electron–ion recombination coefficient (SI unit: m^3/s)
- β_{pn} is the ion–ion recombination coefficient (SI unit: m^3/s)

The above transport equations are fully coupled with Poisson's equation through the electric field and the space charge:

$$\nabla \cdot (\epsilon_r \epsilon_0 \mathbf{E}) = \rho$$

$$\rho = e \sum_i z_i n_i$$

where e is the electric charge.

PHOTOIONIZATION

To model positive gas discharges, it is necessary to compute the photoionization rate. Numerical simulations typically employ the radiative transfer model ([Ref. 2](#)) for this purpose:

$$\nabla^2 S_{\text{ph}}^j - (\lambda_j p_p)^2 S_{\text{ph}}^j = -A_j p_p^2 I_{\text{ph}}$$

where

$$j = 1, 2, 3, \dots$$

$$S_{\text{ph}} = \sum_j S_{\text{ph}}^j$$

$$I_{\text{ph}} = \frac{p_q}{p + p_q} \xi \frac{v_u}{v_i} S_{\text{ion}}$$

where

- S_{ph}^j denotes j^{th} photoionization rate component (SI unit: $1/(\text{m}^3 \cdot \text{s})$)
- p_p is the partial pressure (default value: 150 Torr)
- p is the gas pressure (default value: 760 Torr)
- p_q is the quenching pressure (default value: 30 Torr)
- $\xi v_u/v_i$ is the photoionization parameter (default value: 0.06)
- A_j and λ_j are fitting parameter
- I_{ph} is the effective ionization intensity (SI unit: $1/(\text{m}^3 \cdot \text{s})$)
- S_{ion} is the impact ionization rate (SI unit: $1/(\text{m}^3 \cdot \text{s})$)

Discharges in Liquids

GOVERNING EQUATIONS

The Electric Discharge interface provides built-in charge transport models in liquids. The default model consists of a group of transport equations for each modeled charge carrier ([Ref. 3](#)):

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{w}_i n_i - D_i \nabla n_i) = R_i$$

where

$$i = e, p, n$$

$$z_{e, p, n} = -1, +1, -1$$

$$\mathbf{w}_i = z_i \mu_i \mathbf{E}$$

$$R_e = S_F - \frac{n_e}{\tau_a} - \beta_{ep} n_e n_p$$

$$R_p = S_F - \beta_{ep} n_e n_p - \beta_{pn} n_p n_n$$

$$R_n = \frac{n_e}{\tau_a} - \beta_{pn} n_p n_n$$

$$S_F = \frac{e n_{\text{ioni}} a |\mathbf{E}|}{h} \exp \left[-\frac{\pi^2 m^* a e}{h^2} \left(\frac{\phi_\Delta}{\sqrt{|\mathbf{E}|}} - \frac{\phi_\gamma}{\sqrt{10^6 \text{ V/cm}}} \right)^2 \right]$$

where

- $e, p,$ and n denote electrons, positive ions, and negative ions
- n_i is the number density of the charge carrier (SI unit: $1/\text{m}^3$)
- \mathbf{E} is the electric field (SI unit: V/m)
- z_i denotes the carrier charge (SI unit: 1)
- μ_i denotes the carrier mobility (SI unit: $\text{m}^2/(\text{V}\cdot\text{s})$)
- \mathbf{w}_i is the drift velocity in the electric field (SI unit: m/s)
- D_i is the diffusion coefficient (SI unit: m^2/s)
- R_i is the reaction rate (SI unit: $1/(\text{m}^3\cdot\text{s})$)
- τ_a is the attachment time constant (SI unit: s)
- β_{ep} is the electron–ion recombination coefficient (SI unit: m^3/s)
- β_{pn} is the ion–ion recombination coefficient (SI unit: m^3/s)
- S_F is the field ionization (SI unit: $1/(\text{m}^3\cdot\text{s})$)
- e is the electric charge (SI unit: C)
- n_{ioni} is the number density of ionizable species (SI unit: $1/\text{m}^3$)
- a denotes the molecular separation distance (SI unit: m)
- m^* denotes the effective electron mass (SI unit: kg)
- ϕ_Δ and ϕ_γ are ionization potential parameters (SI unit: V)

The above transport equations are fully coupled with Poisson's equation through the electric field and the space charge:

$$\nabla \cdot (\epsilon_r \epsilon_0 \mathbf{E}) = \rho$$

$$\rho = e \sum_i z_i n_i$$

Bipolar Charge Transport in Solids

The Electric Discharge interface provides built-in charge transport models in solids. The default model consists of a group of transport equations for each modeled charge carrier ([Ref. 4](#)):

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{w}_i n_i - D_i \nabla n_i) = R_i$$

where

$i = e, h, te, th$

$z_{e, h, te, th} = -1, +1, -1, +1$

$\mathbf{w}_i = z_i \mu_i \mathbf{E}$

$$R_e = A_e n_{te} - B_e n_e \left(1 - \frac{n_{te}}{n_{0,te}}\right) - C_1 n_e n_{th} - C_3 n_e n_h$$

$$R_h = A_h n_{th} - B_h n_h \left(1 - \frac{n_{th}}{n_{0,th}}\right) - C_2 n_h n_{te} - C_3 n_e n_h$$

$$R_{te} = -A_e n_{te} + B_e n_e \left(1 - \frac{n_{te}}{n_{0,te}}\right) - C_0 n_{te} n_{th} - C_2 n_h n_{te}$$

$$R_{th} = -A_h n_{th} + B_h n_h \left(1 - \frac{n_{th}}{n_{0,th}}\right) - C_0 n_{te} n_{th} - C_1 n_e n_{th}$$

$$A_e = v_{te} \exp\left(-\frac{e\phi_{te}}{k_B T}\right) \frac{n_{te}}{n_{0,te}}$$

$$A_h = v_{th} \exp\left(-\frac{e\phi_{th}}{k_B T}\right) \frac{n_{th}}{n_{0,th}}$$

where

- $e, h, te,$ and th denote electrons, holes, trapped electrons, and trapped holes
- n_i is the number density of the charge carrier (SI unit: $1/\text{m}^3$)

- \mathbf{E} is the electric field (SI unit: V/m)
- z_i denotes the carrier charge (SI unit: 1)
- μ_i denotes the carrier mobility (SI unit: $\text{m}^2/(\text{V}\cdot\text{s})$)
- \mathbf{w}_i is the drift velocity in the electric field (SI unit: m/s)
- D_i is the diffusion coefficient (SI unit: m^2/s)
- R_i is the reaction rate (SI unit: $1/(\text{m}^3\cdot\text{s})$)
- A_e and A_h are detrapping rate for trapped electrons and trapped holes (SI unit: 1/s)
- B_e and B_h are trapping rate for electrons and holes (SI unit: 1/s)
- v_{te} and v_{th} are attempt-to-escape frequency for trapped electrons and trapped holes (SI unit: 1/s)
- ϕ_{te} and ϕ_{th} are detrapping barrier height for trapped electrons and trapped holes (SI unit: V)
- $n_{0,te}$ and $n_{0,th}$ are density of deep traps for electrons and holes (SI unit: $1/\text{m}^3$)
- k_B is the Boltzmann constant (SI unit: J/K)
- T is the temperature (SI unit: K)
- C_0 is the trapped electron–trapped hole recombination coefficient (SI unit: m^3/s)
- C_1 is the electron–trapped hole recombination coefficient (SI unit: m^3/s)
- C_2 is the trapped electron–hole recombination coefficient (SI unit: m^3/s)
- C_3 is the electron–hole recombination coefficient (SI unit: m^3/s)

The above transport equations are fully coupled with Poisson's equation through the electric field and the space charge:

$$\nabla \cdot (\epsilon_r \epsilon_0 \mathbf{E}) = \rho$$

$$\rho = e \sum_i z_i n_i$$

The above bipolar charge transport equations are based on a two-level transition model, as shown in [Figure 3-3](#).

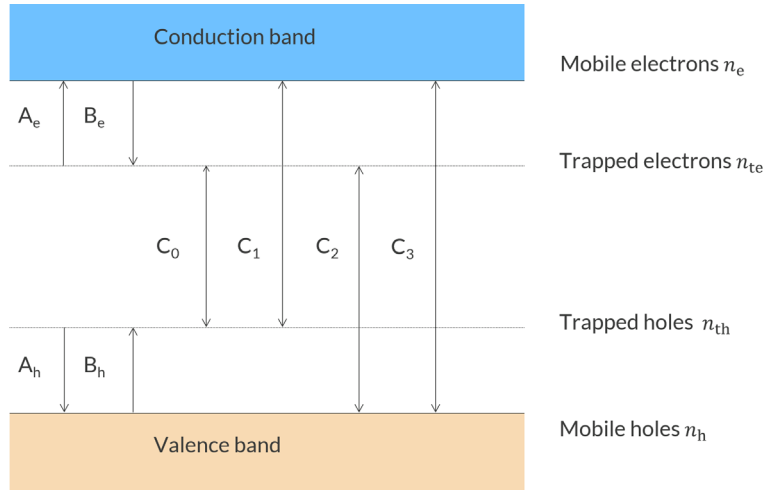


Figure 3-3: Conduction and trapping model for solid dielectrics.

Electrode Boundary Condition

The electrode boundary condition is one of the most critical components in electric discharge modeling. It is used to specify boundary conditions for electric potential and charge carriers.

ELECTRIC POTENTIAL BOUNDARY CONDITIONS

The electric potential boundary condition is implemented as a terminal, where you can either prescribe a voltage or connect to an electrical circuit.

Discharge Current

There are two approaches for computing the discharge current (Ref. 5). The first one views the discharge domain as a two-terminal black box. The total power deposited in the domain is given by

$$P_1 = IV$$

where I is the total current and V is the voltage applied between the two terminals.

The total power can also be computed by integrating the power density over the domain:

$$P_2 = \int_{\Omega} \mathbf{J} \cdot \mathbf{E}$$

where \mathbf{J} is the total current density, including both conduction and displacement components.

By the principle of energy conservation, $P_1 = P_2$. Therefore, the discharge current can be computed as

$$I = \frac{1}{V} \int_{\Omega} \mathbf{J} \cdot \mathbf{E}$$

Another method, more general and used in the electrode feature, involves computing the current flowing through a specific boundary. The current is obtained by boundary integration:

$$I = - \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{J}$$

where \mathbf{n} is the outward-pointing normal vector. Positive and negative currents correspond to the current flowing into and out of the domain, respectively.

For charge transport models, the conduction current density is computed by summing the current flux contributions from each charge carrier:

$$\mathbf{J}_c = e \sum_i \Gamma_i$$

GENERAL CHARGE CARRIER BOUNDARY CONDITIONS

No Diffusive Flux

In most cases, this is the default boundary condition applied on exterior boundaries and prescribes a vanishing flux due to diffusion across the boundary:

$$-\mathbf{n} \cdot (-D\nabla n) = 0$$

This condition implies that convection flux is included, allowing charge carriers to move across the boundary freely. While this boundary condition does not model the detailed interaction of charge carriers with metal surfaces, it is typically a good starting point for most electric discharges, particularly under high pressure-gap products $p \cdot d$ where the discharge within the domain is more significant than that at the boundary.

Number Density

This condition prescribes the number density of charge carriers at the boundary. The number density cannot be set to zero, as the dependent variables are typically the logarithmic values of the number density. Generally, the number density of positive charge carriers is set to a small value at the anode, while for negative charge carriers, it is set to a small value at the cathode.

Open Boundary

This condition allows charge carriers to drift out of the domain but prevents inward flux. It is particularly useful in models where the cathode and anode are not clearly defined, such as when discharges are driven by AC voltages.

No Flux

This boundary condition prescribes a zero total flux (insulation) across the boundary.

Flux

This condition specifies the total charge carrier flux across a boundary, which could occur due to chemical reactions at the boundary. However, when applicable, it is recommended to use built-in surface emission boundary conditions.

SURFACE EMISSION

Surface emission primarily applies to electrons in all media and holes in solids. Three electron emission mechanisms are available.

Secondary Electron Emission

The boundary condition, available for gas domain only, adds secondary electrons generated by the collision of positive ions at the cathode ([Ref. 6](#), p. 71):

$$-\mathbf{n} \cdot \Gamma_e + = \gamma \mathbf{n} \cdot \Gamma_p$$

where γ is the secondary emission coefficient. This is the mechanism responsible for phenomena such as *Trichel pulses*. The interface also provides options to define the boundary condition for outward-drifting carriers.

Field Electron Emission

The field electron emission is only available for gas domain and it is computed as:

$$-\mathbf{n} \cdot \Gamma_e + = \frac{J_F}{e}$$

where the emission current is calculated using the Fowler–Nordheim formula([Ref. 6](#), p. 69):

$$J_F = 6.2 \times 10^{-6} \frac{\sqrt{\epsilon_F/\phi}}{\epsilon_F + \phi} |\mathbf{E}|^2 \exp\left(\frac{-6.85 \times 10^7 \phi^{3/2} \xi}{|\mathbf{E}|}\right) \text{A/cm}^2$$

where ϵ_F is the Fermi energy, ϕ is the work function non-perturbed by the field, and ξ is a correction factor (Ref. 6, p. 70).

Thermionic Emission

The thermionic emission is computed as:

$$-\mathbf{n} \cdot \Gamma_e = \frac{J_{T,e}}{e}$$

where the emission current is calculated using the Dushman–Richardson formula (Ref. 6, p. 68):

$$J_{T,e} = A_0 D T^2 \exp\left(-\frac{e\phi}{k_B T}\right)$$

where A_0 is the Richardson constant, D is a factor that considers the quantum-mechanical effect. For liquid and solid domain, the Schottky effect can be considered.

Charge Transport at Dielectric Interfaces

Charge transport at dielectric interface is critical in many applications. Electric charges can accumulate at the interface, for example, by corona discharge. Space charges at the interface can also drift along the interface surface due to the surface electric field.

For electrostatics, the surface charge is considered through

$$\mathbf{n}_{\text{down}} \cdot (\mathbf{D}_{\text{down}} - \mathbf{D}_{\text{up}}) = -\rho_s$$

where \mathbf{n}_{down} is the outward normal vector from the downside domain and ρ_s is the solution to the following transport equation at the interface:

$$\frac{\partial \rho_s}{\partial t} + \nabla_s \cdot (\sigma_s \mathbf{E}_s) = \mathbf{n}_{\text{up}} \cdot \mathbf{J}_{\text{up}} + \mathbf{n}_{\text{down}} \cdot \mathbf{J}_{\text{down}}$$

where the second term from the left represents the surface conduction. The surface electric field is computed as the negative of the tangential potential gradient. The right-hand side of the equation considers charge transport from bulk materials.

MAGNETIC FIELD DRIFT

When a strong magnetic field is present then the electron mobility can be a tensor:

$$\mu_e^{-1} = \begin{bmatrix} \frac{1}{\mu_{dc}} & -B_z & B_y \\ B_z & \frac{1}{\mu_{dc}} & -B_x \\ -B_y & B_x & \frac{1}{\mu_{dc}} \end{bmatrix}$$

where the inverse of the mobility has been used because the actual expression for the electron mobility cannot be written in a compact form. The quantity μ_{dc} is the electron mobility in the absence of a magnetic field.

CONVECTION

The convection due to a flow field (for gases and liquids) can be easily modeled by adding the flow field to the drift velocity under the electromagnetic field. In general, the flow field has negligible effect on electrons but can have significant effects on ions.

Numerical Stabilization Technique

Transport of charge carriers applications can often result in models with a very high cell Péclet number — that is, systems where drift or convection dominates over diffusion. Numerical stabilization techniques are of paramount importance to obtain physically reasonable results. [The Electric Discharge Interface](#) provides both **Streamline Diffusion** stabilization and **Isotropic Diffusion** stabilization. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.

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Theory for the Arc Discharge Multiphysics Interface

Theory

Arc discharges are widely utilized across various industrial applications due to their unique properties and capabilities. These applications include cutting and welding, where the intense heat of the electric arc melts and fuses materials with high precision. In spraying processes, electric arcs are used to vaporize and deposit materials onto surfaces, enabling the creation of specialized coatings. Arc discharges are also employed in waste destruction technologies, where the high temperatures break down hazardous or complex materials into simpler, safer forms ([Ref. 1](#)).

While electric arcs have many beneficial uses, they are also a significant concern in electrical power systems. In components like circuit breakers, unintended arc formation can lead to equipment damage, power outages, and even safety hazards. Electric arcs in these contexts are undesirable because they can cause rapid degradation of materials, overheating, and potential failure of the entire electrical system.

Accurately simulating and predicting the dynamics of electric arcs is essential. Advanced simulations enable engineers to model the complex interactions that drive arc formation, propagation, and extinction, which in turn helps optimize industrial processes and improve the safety of electrical systems. The Arc Discharge interface is specifically designed to make the modeling of these complex arc discharges more predictable and reliable.

Fully ionized electric arcs are assumed to be under partial to complete local thermodynamic equilibrium (LTE) conditions ([Ref. 1](#)). At a macroscopic level, these kind of plasma can be considered as conductive fluid mixtures, which leads to the magnetohydrodynamics (MHD) equations. The latter combine the Navier–Stokes, heat, and Maxwell’s equations to describe the motion of the conducting fluid in an electromagnetic field.

The Arc Discharge interfaces are based on a set of assumptions that lead to simplifications of the MHD equations:

- The plasma is fully ionized (two-component mixture, that is, electrons and ions).

- The plasma is under local thermodynamic equilibrium (LTE) conditions (the electron temperature T_e is approximately equal to the ion temperature, T_i , under low electric field at atmospheric pressure).
- The plasma is considered to be a locally neutral Newtonian fluid mixture.
- Viscous dissipation and pressure work in the energy equation are neglected.
- The displacement current is negligible (quasistatic approximation, that is, low frequencies).
- Magnetic diffusion dominates induction by fluid motion ($R_{em} \ll 1$).
- The plasma is optically thin.

The magnetic Reynolds number (R_{em}) gives the ratio of induction by fluid motion over the magnetic diffusion

$$R_{em} = \frac{|\nabla \times (\mathbf{u} \times \mathbf{B})|}{|\eta \nabla^2 \mathbf{B}|} \cong \frac{u_0 l_0}{\eta} \quad (3-4)$$

Where the magnetic diffusivity coefficient

$$\eta = (\mu_0 \sigma)^{-1}$$

is the inverse of the product of the plasma conductivity (σ) and vacuum permeability (μ_0). The values u_0 and l_0 are the velocity and length scale of the system under study, respectively.

DOMAIN EQUATIONS

Considering the assumptions stipulated above, the Arc discharges can be described by a set of equations defined in the physics interfaces constituting the different multiphysics interfaces. Note that all the physics features available in the individual physics interfaces are also available to the multiphysics interface in use.

Energy Conservation (Heat Transfer in Fluids Interface and Arc Discharge Heat Source Multiphysics Coupling Feature)

The energy conservation equation is used for the Arc Discharge interface.

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = Q \quad (3-5)$$

The source Q (W/m^3) defined in the Equilibrium Discharge Heat Source multiphysics coupling feature includes three source/sink components:

- Resistive heating (ohmic heating)

$$Q = \mathbf{J} \cdot \mathbf{E} \quad (3-6)$$

The definition of the electric field is:

$$\mathbf{E} = -\left(\nabla V + \frac{\partial \mathbf{A}}{\partial t}\right) \quad (3-7)$$

- Volumetric net radiation loss Q_{rad} defined by the total volumetric emission coefficient, which is a material property from [Ref. 1](#).
- Enthalpy transport (energy carried by the electric current)

$$\frac{\partial}{\partial T} \left(\frac{5k_B T}{2q} \right) (\nabla T \cdot \mathbf{J}) \quad (3-8)$$

Note that the enthalpy transport term prevails, for example, in the boundary layers close to electrodes in a fully ionized electric discharge, [Ref. 1](#).

Momentum Conservation (Laminar Flow Interface)

The momentum conservation equation is expressed as:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot \left[-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \mathbf{F} \quad (3-9)$$

where μ is the dynamic viscosity of the fluid, \mathbf{I} is the identity matrix and

$$\mathbf{F} = \mathbf{J} \times \mathbf{B}$$

the Lorentz force acting on the fluid is defined in the Magnetohydrodynamics coupling feature.

Ampere's Law and Current Conservation (Magnetic and Electric Fields Interface)

The Ampere's Law and Current conservation equations are used for the Arc Discharges interface:

$$\nabla \cdot \mathbf{J} = 0 \quad (3-10)$$

$$\nabla \times \left(\frac{1}{\mu_r \mu_0} \nabla \times \mathbf{A} \right) = \mathbf{J} \quad (3-11)$$

where the total current density is expressed as

$$\mathbf{J} = \sigma \left(-\nabla V - \frac{\partial \mathbf{A}}{\partial t} + \mathbf{u} \times \mathbf{B} \right) \quad (3-12)$$

TRANSPORT PROPERTIES

The above equations require specification of material properties, which are functions of temperature. The Equilibrium Discharge folder in the Material Browser contains properties for density, specific heat, viscosity, thermal conductivity and electric conductivity as a function of temperature up to 25,000 K. Available gases include air, argon, helium, hydrogen, nitrogen, and oxygen. The data is taken from the tables in the Appendix of [Ref. 1](#).

BOUNDARY EQUATIONS

The Arc Discharge interface also includes cooling/heating of electrodes in contact with the electric arc ([Ref. 2](#)).

Ion Bombardment and Thermionic Emission at the Cathode

Positive ions from the plasma are accelerated toward the cathode and generates heat at the electrode surface. As the electrode heats up, more electrons are emitted by thermionic emission, which cause cooling of the cathode. The associated cathode heat flux is defined as:

$$-\mathbf{n} \cdot (-k \nabla T) = -|\mathbf{J}_{\text{elec}}| \phi_s + |\mathbf{J}_{\text{ion}}| V_{\text{ion}} \quad (3-13)$$

Where k is the thermal conductivity (W/(m·K)), ϕ_s is the surface work function of the electrode (V), and V_{ion} is the ionization potential of the plasma (V). The ion current density norm is defined by

$$|\mathbf{J}_{\text{ion}}| = |\mathbf{J} \cdot \mathbf{n}| - |\mathbf{J}_{\text{elec}}| \quad (3-14)$$

where

$$|\mathbf{J} \cdot \mathbf{n}|$$

is the normal current density at the interface and where

$$|\mathbf{J}_{\text{elec}}| = \begin{cases} J_R(T), & |\mathbf{J} \cdot \mathbf{n}| > J_R(T) \\ |\mathbf{J} \cdot \mathbf{n}|, & |\mathbf{J} \cdot \mathbf{n}| \leq J_R(T) \end{cases} \quad (3-15)$$

is the electron current density norm. The latter is defined by Richardson-Dushman current density if the total normal current density is larger than

$$J_R(T) = A_R T^2 \exp\left(-\frac{q\phi_{\text{eff}}}{k_B T}\right) \quad (3-16)$$

Where A_R is the Richardson's constant ($\text{A}/(\text{m}^2 \cdot \text{K}^2)$), q is the electronic charge (C), k_B is the Boltzmann's constant (J/K), and ϕ_{eff} is the effective work function of the surface (V). Note that the ion current density norm $\mathbf{J}_{\text{ion}} = 0$ if the Richardson-Dushman current density is larger than the total normal current at the interface.

Resistive Heating at the Anode

Electron entering the anode generates heat. Following the approach presented in [Ref. 2](#), you can assume that there is no ion current and hence no ion heating at the anode. Accordingly the anode heat flux is defined as:

$$-\mathbf{n} \cdot (-k \nabla T) = |\mathbf{J} \cdot \mathbf{n}| \phi_s \quad (3-17)$$

Where

$$|\mathbf{J} \cdot \mathbf{n}|$$

is the normal current density at the interface, k is the thermal conductivity, and ϕ_s is the surface work function of the anode. Note that all the physics features available in the individual interfaces are also available to the multiphysics interface in use. This include, for instance, radiation heat losses, and wall boundary conditions.

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Theory for the Transport of Charge Carriers Interface

The [Transport of Charge Carriers Interface](#) provides a predefined modeling environment for studying the evolution of charge carriers transported by diffusion and convection as well as migration due to an electromagnetic field. The physics interface can model not only charge carriers such as electrons, holes, and positive and negative ions but also neutrals and their excited states.

In this section:

- [Charge Transport Equation](#)
- [Magnetic Field Drift](#)
- [Numerical Stabilization Technique](#)

Charge Transport Equation

The default node attributed to [The Transport of Charge Carriers Interface](#) models charge transport through diffusion and convection and solves the charge conservation equation for one or more charge carriers i :

$$\begin{aligned}\frac{\partial n_i}{\partial t} + \nabla \cdot \Gamma_i &= R_i \\ \text{where} \\ \Gamma_i &= \Gamma_{ci} + \Gamma_{di} \\ \Gamma_{ci} &= (\mathbf{w}_i + \mathbf{u})n_i \\ \Gamma_{di} &= -D_i \nabla n_i \\ \mathbf{w}_i &= f(z_i, \mu_i, \mathbf{E}, \mathbf{B}, \mathbf{u})\end{aligned}\tag{3-18}$$

[Equation 3-18](#) in its form above includes drift in electric and magnetic fields, convection in flow fields, and diffusion due to charge carrier density gradients. See more details in [Transport Mechanisms](#).

- n_i is the number density of the charge carrier (SI unit: $1/\text{m}^3$)
- Γ_i is the total flux (SI unit: $1/(\text{m}^2 \cdot \text{s})$)
- Γ_{ci} is the convective flux (SI unit: $1/(\text{m}^2 \cdot \text{s})$)

- Γ_{di} is the diffusive flux (SI unit: $1/(m^2 \cdot s)$)
- \mathbf{w}_i is the drift velocity in electromagnetic fields (SI unit: m/s)
- z_i denotes the carrier charge (SI unit: 1)
- μ_i denotes the carrier mobility (SI unit: $m^2/(V \cdot s)$)
- D_i denotes the carrier diffusion coefficient (SI unit: m^2/s)
- \mathbf{E} is the electric field (SI unit: V/m)
- \mathbf{B} is the magnetic field (SI unit: T)
- \mathbf{u} is the flow field velocity vector (SI unit: m/s)
- R_i is a reaction rate expression for the species (SI unit: $mol/(m^3 \cdot s)$)

The electric field \mathbf{E} , magnetic field \mathbf{B} , and the velocity field \mathbf{u} can be expressed analytically or obtained from coupling the physics interface to one that solves for the field, such as *Electrostatics*, *Magnetic Fields*, and *Laminar Flow*, respectively.

On the right-hand side of the mass balance equation (Equation 3-18), R_i represents a source or sink term, typically due to chemical reactions. To specify R_i , another node must be added to [The Transport of Charge Carriers Interface](#) — the **Reaction** node for example, which includes an input field for specifying a reaction expression using the variable names of all participating species.

Magnetic Field Drift

When a strong magnetic field is present then the electron mobility can be a tensor:


$$\mu_e^{-1} = \begin{bmatrix} \frac{1}{\mu_{dc}} & -B_z & B_y \\ B_z & \frac{1}{\mu_{dc}} & -B_x \\ -B_y & B_x & \frac{1}{\mu_{dc}} \end{bmatrix}$$

where the inverse of the mobility has been used because the actual expression for the electron mobility cannot be written in a compact form. The quantity μ_{dc} is the electron mobility in the absence of a magnetic field.

Numerical Stabilization Technique

Transport of charge carriers applications can often result in models with a very high cell Péclet number — that is, systems where drift or convection dominates over diffusion. Numerical stabilization techniques are of paramount importance to obtain physically reasonable results. [The Transport of Charge Carriers Interface](#) provides both streamline diffusion stabilization and isotropic diffusion stabilization. See more details in [Numerical Stabilization](#) in the *COMSOL Multiphysics Reference Manual*.

AC/DC Interfaces


This chapter describes the usage and theory for the physics interfaces found under the AC/DC branch ().

In this chapter:

- [The Electrostatics Interface](#)
- [The Magnetic and Electric Fields Interface](#)
- [The Electrical Circuit Interface](#)
- [Theory for the Electrostatics Interface](#)
- [Theory for the Magnetic and Electric Fields Interface](#)
- [Theory for the Electrical Circuit Interface](#)

See [The Electromagnetics Interfaces](#) in the *COMSOL Multiphysics Reference Manual* for other AC/DC interface and feature node settings.

The Electrostatics Interface

The **Electrostatics (es)** interface (), found under the **AC/DC > Electric Fields and Currents** branch when adding a physics interface, is used to compute the electric field, electric displacement field, and potential distributions in dielectrics under conditions where the electric charge distribution is explicitly prescribed. The formulation is stationary except for when it is used together with other physics interfaces. Eigenfrequency, frequency-domain, small-signal analysis, and time-domain modeling are supported in all space dimensions.

The physics interface solves Gauss' law for the electric field using the scalar electric potential as the dependent variable.

Charge Conservation is the main node, which adds the equation for the electric potential and has a Settings window for defining the constitutive relation for the electric displacement field and its associated properties such as the relative permittivity.

When this physics interface is added, these default nodes are also added to the **Model Builder — Free Space, Zero Charge** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and space charges. You can also right-click **Electrostatics** to select physics features from the context menu.

Physics-Controlled Mesh

The physics-controlled mesh is controlled from the **Mesh** node's **Settings** window (if the **Sequence type** is **Physics-controlled mesh**). There, in the table in the **Physics-Controlled Mesh** section, find the physics interface in the **Contributor** column and select or clear the checkbox in the **Use** column on the same table row for enabling (the default) or disabling contributions from the physics interface to the physics-controlled mesh.

Information from the physics, such as the presence of an infinite elements domain or periodic condition, will be used to automatically set up an appropriate meshing sequence.



In the *COMSOL Multiphysics Reference Manual* see the [Physics-Controlled Mesh](#) section for more information about how to define the physics-controlled mesh.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `es`.

CROSS-SECTION AREA (1D COMPONENTS)

For 1D components, enter a default value for the **Cross-section area** A (SI unit: m^2). The default value of 1 is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components. See also [Change Cross Section](#).

THICKNESS (2D COMPONENTS)

For 2D components, enter a default value for the **Out-of-plane thickness** d (SI unit: m). The default value of 1 is typically not representative for a thin dielectric medium, for example. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components. See also [Change Thickness \(Out-of-Plane\)](#).

DEPENDENT VARIABLES

The dependent variable is the **Electric potential** V . You can change its name, which changes both the field name and the variable name. If the new name coincides with the name of another dependent variable in the model, the physics interfaces shares degrees of freedom. The new name must not coincide with the name of a field of another type or with a component name belonging to some other field.

DISCRETIZATION

Select the shape order for the **Electric potential** dependent variable — **Linear**, **Quadratic** (the default), **Cubic**, **Quartic**, or **Quintic**. For more information about the **Discretization**

section, see [Settings for the Discretization Sections](#) in the *COMSOL Multiphysics Reference Manual*.



In the *COMSOL Multiphysics Reference Manual*, see [Table 2-4](#) for links to common sections and [Table 2-5](#) to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.



Electric Sensor: Application Library path
COMSOL_Multiphysics/Electromagnetics/electric_sensor

Domain, Boundary, Edge, Point, and Pair Nodes for the Electrostatics Interface

The Electrostatics interface has these domain, boundary, edge, point, and pair nodes available.

ABOUT THE BOUNDARY CONDITIONS

The relevant physics interface condition at interfaces between different media is

$$\mathbf{n}_2 \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

In the absence of surface charges, this condition is fulfilled by the natural boundary condition

$$\mathbf{n} \cdot [(\epsilon_0 \nabla V - \mathbf{P})_1 - (\epsilon_0 \nabla V - \mathbf{P})_2] = -\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0$$

AVAILABLE NODES

These nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users). Also see [Table 4-1](#) for a list of interior and exterior boundary conditions, including edge, point, and pair availability.



In general, to add a node, go to the **Physics** toolbar no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Change Cross Section
- Change Thickness (Out-of-Plane)
- Charge Conservation
- Charge Conservation, Piezoelectric^{1,2}
- Conduction Loss (Time-Harmonic)
- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- External Surface Charge Accumulation
- Floating Potential
- Ground
- Initial Values
- Line Charge
- Line Charge (on Axis)
- Line Charge (Out-of-Plane)
- Periodic Condition
- Point Charge
- Point Charge (on Axis)
- Space Charge Density
- Surface Charge Accumulation
- Surface Charge Density
- Symmetry Plane (for Electric Field)
- Terminal
- Thin Low Permittivity Gap
- Zero Charge (the default boundary condition)

¹This feature is available with the Piezoelectricity multiphysics interface.

²Requires either the Acoustics Module, MEMS Module, or Structural Mechanics Module.

Table 4-1 lists the interior and exterior boundary conditions available with this physics interface. It also includes edge, point, and pair availability.

TABLE 4-1: INTERIOR AND EXTERIOR BOUNDARY CONDITIONS (INCLUDING EDGE, POINT, AND PAIR AVAILABILITY) FOR THE ELECTROSTATICS INTERFACE.

NODE	INTERIOR	EXTERIOR	ALSO AVAILABLE FOR
Change Cross Section	x	x	pairs
Change Thickness (Out-of-Plane)	x	x	pairs
Dielectric Shielding	x	x	pairs
Distributed Capacitance		x	pairs
Electric Displacement Field	x	x	pairs
Electric Potential	x	x	edges, points, and pairs
External Surface Charge Accumulation		x	pairs
Floating Potential	x	x	pairs

TABLE 4-1: INTERIOR AND EXTERIOR BOUNDARY CONDITIONS (INCLUDING EDGE, POINT, AND PAIR AVAILABILITY) FOR THE ELECTROSTATICS INTERFACE.

NODE	INTERIOR	EXTERIOR	ALSO AVAILABLE FOR
Ground	x	x	edges, points, and pairs
Periodic Condition		x	not applicable
Surface Charge Accumulation	x		not applicable
Surface Charge Density	x	x	pairs
Symmetry Plane		x	not applicable
Terminal	x	x	domains
Thin Low Permittivity Gap	x		not applicable
Zero Charge (the default)	x	x	pairs



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the model that is valid on the axial symmetry boundaries only. There are also **Line Charge (on Axis)** and **Point Charge (on Axis)** available.



In the *COMSOL Multiphysics Reference Manual*, see [Table 2-4](#) for links to common sections and [Table 2-5](#) to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Free Space

For electromagnetic modeling, it is quite common for the fields to extend into the environment of the device in question. It is therefore important not only to model the device itself, but also its surroundings. Typically, this is done by adding a box or sphere around the device's geometry.

The default **Free Space** node is used to specify the physical conditions in close proximity to the device — typically in air or vacuum. It adds a **Charge Conservation** governing equation using the **Relative permittivity** constitutive relation with the permittivity ϵ_r set to one.

The **Free Space** feature provides a canvas on top of which other features can be added to locally specify material properties and excitation forms.

Charge Conservation

The **Charge Conservation** node adds the equations for charge conservation according to Gauss' law for the electric displacement field. It provides an interface for defining the constitutive relation and its associated properties such as the relative permittivity.

There are two types of **Charge Conservation** available; **Charge Conservation in Solids** and **Charge Conservation in Fluids**. This distinction decides how materials behave and how material properties are interpreted when the mesh is deformed.

Charge Conservation in Solids applies to materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame).

Charge Conservation in Fluids applies to materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined.



In COMSOL versions **6.2** and earlier, this **Solids/Fluids** distinction was controlled within the **Charge Conservation** node by specifying **Solid/Nonsolid** in the **Material type** setting.

CONSTITUTIVE RELATION \mathbf{D} - \mathbf{E}

Select a **Dielectric model** to describe the macroscopic properties of the medium (relating the electric displacement \mathbf{D} with the electric field \mathbf{E}) and the applicable material properties, such as the relative permittivity. Note that **Charge Conservation in Fluids** uses only **Relative permittivity** or **Polarization**. The other constitutive relations are only accessible in **Charge Conservation in Solids**. Select:

- **Relative permittivity** (the default) to use the constitutive relation $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$. Then the default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. The default is 1.
- **Polarization** to use the constitutive relation $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$. Then enter the components based on space dimension for the **Polarization** vector \mathbf{P} (SI unit: C/m²). The defaults are 0 C/m².
- **Remanent electric displacement** to use constitutive relation $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E} + \mathbf{D}_r$, where \mathbf{D}_r is the remanent displacement (the displacement when no electric field is present). Then the default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter

values or expressions in the field or matrix. Then enter the components based on space dimension for the **Remanent electric displacement \mathbf{D}_r** (SI unit: C/m²). The defaults are 0 C/m².

Conduction Loss (Time-Harmonic)



This feature requires either the Acoustics Module, or MEMS Module, or Structural Mechanics Module. See the individual documentation for information.

The **Conduction Loss (Time-Harmonic)** subnode to **Charge Conservation** allows you to model possible conductive losses in a dielectric material. The effect is only active in an Eigenfrequency or Frequency Domain study.

CONDUCTION CURRENT

By default, the **Electric conductivity σ** for the media is defined **From material**. You can also select **User defined** or **Linearized resistivity**.

- For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** depending on the characteristics of the electric conductivity, and then enter values or expressions for the **Electric conductivity σ** in the field or matrix.
- For **Linearized resistivity** the default **Reference temperature T_{ref}** , and **Resistivity temperature coefficient α** , and **Reference resistivity ρ_0** are taken **From material**, which means that the values are taken from the domain (or boundary) material. T is the current temperature, which can be a value that is specified as a model input or the temperature from a heat transfer interface. The definition of the temperature field appears in the **Model Inputs** section.

LOCATION IN USER INTERFACE

Context Menus

Electrostatics > Charge Conservation > Conduction Loss (Time-Harmonic)

Ribbon

Physics tab with **Charge Conservation** node selected in the model tree:

Attributes > Conduction Loss (Time-Harmonic)

Initial Values

The **Initial Values** node adds an initial value for the electric potential V that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Electric potential** V (SI unit: V). The default value is 0 V.

Space Charge Density

The **Space Charge Density** node adds a space charge density ρ , which appears on the right-hand side of the equation that the physics interface defines.

SPACE CHARGE DENSITY

Enter a value or expression for the **Space charge density** ρ_v (SI unit: C/m³). The default is 0 C/m³.

Zero Charge

The **Zero Charge** node adds the condition that there is zero charge on the boundary so that $\mathbf{n} \cdot \mathbf{D} = 0$. This boundary condition is also applicable at symmetry boundaries where the potential is known to be symmetric with respect to the boundary. This is the default boundary condition at exterior boundaries. At interior boundaries, it means that no displacement field can penetrate the boundary and that the electric potential is discontinuous across the boundary.

Ground

The **Ground** node implements ground (zero potential) as the boundary condition $V = 0$.

Ground means that there is a zero potential on the boundary. This boundary condition is also applicable at symmetry boundaries where the potential is known to be antisymmetric with respect to the boundary.


For some physics interfaces, also select additional **Ground** nodes from the **Edges** (3D components) or **Points** (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the Symmetry axis.

BOUNDARY, EDGE, OR POINT SELECTION



Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

Electric Potential

The **Electric Potential** node provides an electric potential V_0 as the boundary condition $V = V_0$.

Because the electric potential is being solved for in the physics interface, the value of the potential is typically defined at some part of the geometry. For some physics interfaces, also select additional **Electric Potential** nodes from the **Edges** (3D components) or **Points** (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the symmetry axis.

BOUNDARY, EDGE, OR POINT SELECTION




Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

ELECTRIC POTENTIAL

Enter the value or expression for the **Electric potential** V_0 (SI unit: V). The default is 0 V.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

Surface Charge Density

The **Surface Charge Density** node provides the following surface-charge boundary condition for exterior boundaries (left) and interior boundaries (right):

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s, \quad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

Specify the surface charge density ρ_s at an outer boundary or at an interior boundary between two nonconducting media.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** in the **Physics** toolbar. For more information, see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

SURFACE CHARGE DENSITY

Enter the value or expression for the **Surface charge density** ρ_s (SI unit: C/m²).

External Surface Charge Accumulation

The **External Surface Charge Accumulation** node implements the boundary condition

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s$$

where ρ_s is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density on the wall and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density on the wall, which are feature inputs.

MATERIAL TYPE

The **Material type** setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select **Solid** for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select **Nonsolid** for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select **From material** to pick up the corresponding setting from the domain material on each domain.

EXTERNAL SURFACE CHARGE ACCUMULATION

Enter values or expressions for the **Normal ion current density** $\mathbf{n} \cdot \mathbf{J}_i$ (SI unit: A/m²) and the **Normal electron current density** $\mathbf{n} \cdot \mathbf{J}_e$ (SI unit: A/m²).

Symmetry Plane (for Electric Field)

The **Symmetry Plane** node adds a boundary condition that represents symmetry or antisymmetry in the electric field, depending on which option is chosen.

SYMMETRY TYPE

Choose between **Symmetry** and **Antisymmetry** for the electric field. If **Symmetry** is chosen, the boundary condition is

$$\mathbf{n} \cdot \mathbf{E} = 0$$

which states that the normal component of the electric field is zero. If **Antisymmetry** is chosen, the boundary condition becomes

$$\mathbf{n} \times \mathbf{E} = 0$$

which states that the tangential component of the electric field is zero.

Electric Displacement Field

The **Electric Displacement Field** node adds the following electric-displacement boundary condition:

$$\mathbf{n} \cdot \mathbf{D} = \mathbf{n} \cdot \mathbf{D}_0$$

It specifies the normal component of the electric displacement field at a boundary.

ELECTRIC DISPLACEMENT FIELD

Enter the coordinates of the **Boundary electric displacement field \mathbf{D}_0** (SI unit: C/m²).

Periodic Condition

The **Periodic Condition** node defines periodicity or antiperiodicity between two boundaries. If required, activate periodic conditions on more than two boundaries, in which case the Periodic Condition tries to identify two separate surfaces that can each consist of several connected boundaries. For more complex geometries, it might be necessary to use the **Destination Selection** section, which you activate by right-clicking the **Periodic Condition** node and select **Manual Destination Selection**. With that section,

the boundaries which constitute the source and destination surfaces can be manually specified.



When this feature is used in conjunction with a [Sector Symmetry](#) feature on connected boundaries, wherever the sector symmetry boundaries connect with the periodic boundaries, the same periodic condition feature cannot be used on both sides. At least two periodic condition features are required for the model to compute correctly.

BOUNDARY SELECTION



The software usually automatically identifies the boundaries as either source boundaries or destination boundaries, as indicated in the selection list. This works fine for cases like opposing parallel boundaries. In other cases, right-click **Periodic Condition** and select **Manual Destination Selection** to control the destination. By default it contains the selection that COMSOL Multiphysics identifies.

When using nonconforming meshes on the source and destination of a periodic boundary pair, for numerical stability, a finer mesh should be applied on the destination side. Use conforming meshes if possible.

DESTINATION SELECTION


This section is available for specifying the destination boundaries, if needed, when the **Manual Destination Selection** option is selected in the context menu for the **Periodic Condition** node. You can only select destination boundaries from the union of all source and destination boundaries.

PERIODIC CONDITION


Select a **Type of periodicity** — **Continuity** (the default), **Antiperiodicity**, or **Floquet periodicity**. Select:

- **Continuity** to make the potential periodic (equal on the source and destination).
- **Antiperiodicity** to make it antiperiodic.
- **Floquet periodicity** (only available with products supporting piezoelectric modeling). Specify the components of the **k-vector for Floquet periodicity** \mathbf{k}_F (SI unit: rad/m).

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

ORIENTATION OF SOURCE

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog. For information about the **Orientation of Source** section, see [Orientation of Source and Destination](#) in the *COMSOL Multiphysics Reference Manual*.

ORIENTATION OF DESTINATION

This section appears if the setting for **Transform to intermediate map** in the **Orientation of Source** section is changed from the default value, **Automatic**, and **Advanced Physics Options** is selected in the **Show More Options** dialog. For information about the **Orientation of Destination** section, see [Orientation of Source and Destination](#) in the *COMSOL Multiphysics Reference Manual*.

Thin Low Permittivity Gap

Use the **Thin Low Permittivity Gap** node

$$\mathbf{n} \cdot \mathbf{D}_1 = \frac{\epsilon_0 \epsilon_r}{d} (V_1 - V_2)$$
$$\mathbf{n} \cdot \mathbf{D}_2 = \frac{\epsilon_0 \epsilon_r}{d} (V_2 - V_1)$$

to model a thin gap of a material with a small permittivity compared to the adjacent domains. The layer has the thickness d and the relative permittivity ϵ_r . The indices 1 and 2 refer to the two sides of the boundary.

THIN LOW PERMITTIVITY GAP

The default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. For **User defined**, enter a different value or expression. Enter a **Thickness** d (SI unit: m). The default is 5 mm.

Surface Charge Accumulation

On interior boundaries, the **Surface Charge Accumulation** node implements the boundary condition

$$\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

where ρ_s is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density on the wall and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density on the wall.

SURFACE CHARGE ACCUMULATION

Enter the values or expressions for the **Normal ion current density** $\mathbf{n} \cdot \mathbf{J}_i$ (SI unit: A/m²) and the **Normal electron current density** $\mathbf{n} \cdot \mathbf{J}_e$ (SI unit: A/m²).

Dielectric Shielding

The **Dielectric Shielding** node adds dielectric shielding as a boundary condition. It describes a thin layer with thickness d_s and a bulk relative permittivity ϵ_r that shields the electric field:

$$\mathbf{n} \cdot \mathbf{D} = -\nabla_t \cdot \epsilon_0 \epsilon_{rs} d_s \nabla_t V$$

Use this boundary condition when approximating a thin domain with a boundary to reduce the number of mesh elements.

MATERIAL TYPE


The **Material type** setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select **Solid** for materials whose properties change as functions of material strain, material orientation and other variables evaluated in a material reference configuration (material frame). Select **Nonsolid** for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select **From material** to pick up the corresponding setting from the domain material on each domain.

ELECTRIC SHIELDING

The default is to take the **Relative permittivity** ϵ_r (dimensionless) values **From material**. It takes it from the adjacent domains if not explicitly defined. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. Enter a **Surface thickness** d_s (SI unit: m) of the shielding. The default is 1 m.

Terminal

The **Terminal** node provides a boundary or domain condition for connection to external circuits, to transmission lines, or with a specified voltage or charge. By specifying zero charge, a floating potential condition is obtained.

An operation called **Split by Connectivity** () is available by right-clicking the parent node. The operation is useful when there are several terminal domains or boundaries that are not geometrically connected. Clicking the operation node will automatically generate several **Terminal** nodes where each selection is geometrically connected.

The **Terminal** node also enables the computation of the lumped parameters of the system, such as capacitance..

TERMINAL

Specify the terminal properties. Enter a unique **Terminal name** that will be used to identify the global variables (such as the terminal voltage or current) that are defined by the terminal. The **Terminal name** can contain alphanumeric characters, but it should be numeric when performing terminal sweeps.

Select a **Terminal type** — **Charge** (the default), **Voltage**, **Circuit**, **Terminated (power)**, or **Terminated (voltage)**. Select:

- **Charge** to prescribe the total charge deposited on the terminal boundaries. Enter the total charge Q_0 . The default is 0 C, which corresponds to a uncharged floating electrode.
- **Voltage** to specify a fixed electric potential at the terminal. Enter an electric potential V_0 . The default is 1 V.
- **Circuit** to specify a terminal connected to an Electrical Circuit interface that models an external circuit. The Terminal node provides a current-voltage characteristic to the circuit.
- **Terminated (power)** to connect the terminal to an impedance that might represent a load or a transmission line. When **Terminated (power)** is selected, the scattering parameters (S-parameters) are computed. The **Terminated (power)** setting can only be used in frequency-domain studies.
 - Enter a **Terminal power** P_0 to specify the input power at this terminal from the transmission line. This excitation can be toggled using a port sweep.
 - Select an option from the **Characteristic impedance from** list to define the value of the impedance — **Physics interface** or **User defined**. For **Physics interface**, the **Reference impedance** Z_{ref} defined in the **Settings** window for the physics under

Sweep Settings is used. For **User defined**, enter a specific impedance Z_{ref} for this terminal. The default is $50 \, \Omega$.

- **Terminated (voltage)** to connect the terminal to an impedance that might represent a load or a transmission line. The **Terminated (voltage)** option is essentially the same as **Terminated (power)**, with the power defined as: $P_0 = 0,5 \cdot |V_0|^2 / Z_{\text{ref}}$.

When **Terminal type** is selected as **Charge** or **Voltage**, a contribution can be added as **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.


Initial values

The initial values subsection is used to provide initial values for the internal state variables in the Terminal. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

The **Initial value for voltage** is available for all Terminal types except Voltage. Enter an **Initial value for voltage** V_{init} .

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the terminal when the circuit is connected. Enter an **Initial value for charge** Q_{init} .

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

Floating Potential

The **Floating Potential** node is used when modeling a metallic electrode at floating potential. It applies a constant voltage V_0 on the boundary (for domain features, this is the boundary enclosing the selected domain), such that the total normal electric displacement field \mathbf{D} equals a specific charge Q_0 :

$$V = V_0$$

$$\int_{\partial\Omega} (\mathbf{D} \cdot \mathbf{n}) dS = Q_0,$$

where $\partial\Omega$ represents the boundary and \mathbf{n} refers to the surface normal. The constant boundary voltage implies the tangential electric field equals zero; the electric field will be perpendicular to the boundary:

$$\begin{aligned} -\nabla_t V &= \mathbf{E}_t = 0 \\ \mathbf{n} \times \mathbf{E} &= 0. \end{aligned}$$

In case of $Q_0 = 0$ (the default case), the boundary will behave as an unconnected, neutrally charged, good conductor under electrostatic conditions (a floating equipotential). Although locally the displacement field may vary, the total electric displacement field entering or leaving the boundary equals zero.

If the floating potential touches a point, boundary, or domain feature that is not floating (a **Terminal** or **Ground** feature), the floating potential will acquire that feature's potential. If the floating potential is set to a certain charge, or connected to a circuit, it behaves like a terminal.

FLOATING POTENTIAL

The **Floating potential identifier** text area shows the unique identifier for the floating potential feature. It is used to identify the global variables created by the node, such as the voltage. The **Floating potential group** checkbox in the **Settings** window for **Floating Potential** controls how potentials are assigned to boundary segments in the feature's boundary selection. If this checkbox is not selected, a single potential is applied to all boundaries in the selection. If the checkbox is selected, each group of contiguous boundaries in the selection is given a unique potential. This simplifies the setup of models with many floating electrodes. The values of the potential at each group of boundaries are then made available in postprocessing, collected in a vector variable.

The following options are not available if the **Floating potential group** checkbox is selected. Select a specification for the **Electric charge** — choose **User defined** to specify a total **Charge** Q_0 deposited on the surface. Select **Circuit** to connect the floating potential to an Electrical Circuit.


Initial Values

The initial values subsection is used to provide initial values for the internal state variables in the Floating potential. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

Enter an **Initial value for voltage** V_{init} .

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the floating potential when the circuit is connected. Enter an **Initial value for charge** Q_{init} .

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

Distributed Capacitance

The **Distributed Capacitance** node adds a distributed capacitance boundary condition according to the following equations for exterior boundaries:

$$-\mathbf{n} \cdot \mathbf{D} = \epsilon_0 \epsilon_r \frac{V_{\text{ref}} - V}{d_s}$$

Use this boundary condition to model a thin sheet or film of a dielectric material. The sheet has the relative permittivity ϵ_r and the surface thickness d_s , and it is connected to the reference potential V_{ref} .

DISTRIBUTED CAPACITANCE

Enter the values or expressions for **Relative permittivity** ϵ_r (dimensionless), **Surface thickness** d_s (SI unit: m), and **Reference potential** V_{ref} . The default value for the surface thickness is 10^{-3} m (1 mm) and 0 V for the reference potential.

Line Charge

For 3D components, use the **Line Charge** node to specify line charges along the edges of a geometry. Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

EDGE SELECTION



Beware that constraining the potential on edges usually yields a current outflow that is mesh dependent.

LINE CHARGE

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.



Line Charge (on Axis) and Line Charge (Out-of-Plane)

Line Charge (on Axis)

For 2D axisymmetric components, use the **Line Charge (on Axis)** node to specify line charges along the symmetry axis.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

LINE CHARGE (ON AXIS)

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.



Line Charge and Line Charge (Out-of-Plane)

Line Charge (Out-of-Plane)

For 2D and 2D axisymmetric components, points are selected and this is the same as a line out-of-plane.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

Use the **Line Charge (Out-of-Plane)** node to specify line charges along the points of a geometry for 2D and 2D axisymmetric components.

POINT SELECTION



Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

LINE CHARGE (OUT-OF-PLANE)

Enter a value or expression to apply a **Line charge** Q_L (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.



[Line Charge](#) and [Line Charge \(on Axis\)](#)

Point Charge

The **Point Charge** node adds a point source to 3D components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

POINT SELECTION



Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT CHARGE

Enter a value or expression to apply a **Point charge** Q_P (SI unit: C) to points. This source represents an electric displacement field flowing out of the point. The default is 0 C.



[Point Charge \(on Axis\)](#) and [Line Charge \(Out-of-Plane\)](#)

Point Charge (on Axis)

The **Point Charge (on Axis)** node adds a point source to 2D axisymmetric components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

POINT SELECTION



Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT CHARGE (ON AXIS)

Enter a value or expression to apply a **Point charge** Q_P (SI unit: C) to points on an axis. This source represents an electric displacement field flowing out of the point. The default is 0 C.



[Point Charge](#) and [Line Charge \(Out-of-Plane\)](#)

Change Cross Section

This node is available with 1D components. This setting overrides the global **Cross-Section Area** setting made in any physics interface that uses this feature. For 2D components, see [Change Thickness \(Out-of-Plane\)](#).

Use the **Change Cross Section** node to set the cross-section area for specific geometric entities.

CHANGE CROSS SECTION

Enter a value or expression for the **Cross-section area** A . The default value of one unit area is typically not representative for the actual domain. Instead, it describes a unit area that makes the 1D equation identical to the equation used for 3D components.

Change Thickness (Out-of-Plane)

This node is available for 2D components. This setting overrides the global **Thickness** setting made in any physics interface that uses this node. For 1D components, see [Change Cross Section](#).

Use the **Change Thickness (Out-of-Plane)** node to set the out-of-plane thickness for specific geometric entities.

CHANGE THICKNESS (OUT-OF-PLANE)

Enter a value or expression for the **Out-of-plane thickness** d (SI unit: m). The default value is, in most cases, 1 unit length, which is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components.

Charge Conservation, Piezoelectric



This feature is available with the Piezoelectricity interface, which requires either the Acoustics Module, or MEMS Module, or Structural Mechanics Module. See the individual documentation for information.

The **Charge Conservation, Piezoelectric** node is normally used together with a **Piezoelectric Effect** multiphysics coupling node and a corresponding **Piezoelectric Material** node in the **Solid Mechanics** interface. The node is added by default to the **Electrostatics** interface when adding a Piezoelectricity interface. It is also available from the context menu (right-click the **Electrostatics** interface parent node) or from the **Physics** toolbar.



When the **Charge Conservation, Piezoelectric** node is added to the electrostatics interface in the absence of an active **Piezoelectric Effect** multiphysics coupling node, the material behaves similarly to a [Charge Conservation](#) node, with electric properties corresponding to the relative permittivity entered (see below). The piezoelectric effect is *not* included in the corresponding equation system.

ELECTRIC DISPLACEMENT

If the node is used together with an active **Piezoelectric Effect** multiphysics coupling node, then these settings are locked. Note that if they are unlocked, then the material

behaves like a dielectric and *not* a piezoelectric. In this case, the default is to take the **Relative permittivity** ϵ_{TS} (dimensionless) values **From material**. For **User defined**, select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix.

Electrostatic Point Dipole

Add an **Electrostatic Point Dipole** node to 3D and 2D components. Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or click **Harmonic Perturbation** in the **Physics** toolbar. For more information see [Harmonic Perturbation — Exclusive and Contributing Nodes](#) in the *COMSOL Multiphysics Reference Manual*.

The **Electrostatic Point Dipole** represents the limiting case of zero separation distance between two equally strong point sources of opposing signs while maintaining the product between separation distance and source strength at a fixed value (p). The dipole moment is a vector entity with positive direction from the negative charge to the positive one.


ELECTROSTATIC POINT DIPOLE

Select a **Dipole specification** — **Magnitude and direction** (the default) or **Electric dipole moment**.

For **Magnitude and direction** enter coordinates for the **Electric dipole moment direction** \mathbf{n}_p (dimensionless) and the **Electric dipole moment, magnitude** p .

For **Electric dipole moment** enter coordinates for the **Electric dipole moment** \mathbf{p} .

The Magnetic and Electric Fields Interface

The **Magnetic and Electric Fields (mef)** interface () is found under the **AC/DC > Electromagnetic Fields > Vector Formulations** branch when adding a physics interface, is used to compute magnetic field and current distributions when the exciting current is driven by an applied voltage. Stationary, time-dependent modeling are supported in 2D and 3D.

The physics interface solves Maxwell's equations formulated using the magnetic vector potential and the scalar electric potential as the dependent variables.

Use the Magnetic and Electric Fields interface when the current continuity equation is needed everywhere in the simulation domain.

The main node is the **Ampère's Law and Current Conservation** feature, which adds the equation for the electric potential and magnetic vector potential and provides an interface for defining the constitutive relations and their associated properties such as the relative permeability, relative permittivity, and electric conductivity.

The **Ampère's Law and Current Conservation** feature can be overridden with an **Ampère's Law** feature or a **Coil** feature, that are identical to the ones in the **Magnetic Fields** interface, removing the electric potential and the current conservation equation from the selected domains.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Free Space, Magnetic Insulation** (the default boundary condition for the magnetic vector potential), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and external currents. You can also right-click **Magnetic and Electric Fields** to select physics features from the context menu.

Physics-Controlled Mesh

The physics-controlled mesh is controlled from the **Mesh** node's **Settings** window (if the **Sequence type** is **Physics-controlled mesh**). There, in the table in the **Physics-Controlled Mesh** section, find the physics interface in the **Contributor** column and select or clear the checkbox in the **Use** column on the same table row for enabling (the default) or disabling contributions from the physics interface to the physics-controlled mesh.

Information from the physics, such as the presence of an infinite elements domain or periodic condition, will be used to automatically set up an appropriate meshing sequence.



In the *COMSOL Multiphysics Reference Manual* see the [Physics-Controlled Mesh](#) section for more information about how to define the physics-controlled mesh.



Except where described below, most **Settings** windows are the same as for the Magnetic Fields, Electrostatics, and Electric Currents interfaces. Also see [About the Magnetic and Electric Fields Interface Boundary Conditions](#) for more information.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the `name` string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `mef`.

BACKGROUND FIELD

The only option available from the **Solve for** list is **Full field**.

COMPONENTS



For 2D and 2D axisymmetric components, select **Components** — **Out-of-plane vector potential** (the default), **In-plane vector potential**, or **Three-component vector potential**. From the practical viewpoint this choice is equivalent to deciding in what directions the electric current is allowed to flow (out-of-plane currents, in-plane currents or currents flowing in all three coordinate directions).

THICKNESS



Enter a value or expression for the **Out-of-plane thickness** d . The default value of 1 unit length is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components.

ERROR CHECK

To display this section, click the **Show More Options** button () and select **Advanced Physics Options**.

When the **Check applicability of features in study** checkbox is selected, any features that are incompatible with the study will generate an error message when trying to solve or show the default solver. No solver will be generated. Deselect it and you will be able to run the model, possibly with runtime errors instead. It is available to allow the advanced user to tweak any feature and use it outside of its intended study scope.

DEPENDENT VARIABLES

The dependent variables (field variables) are for the **Electric potential** V and **Magnetic vector potential** A . The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

Select the shape order for the **Magnetic vector potential** dependent variable — **Linear**, **Quadratic** (the default), or **Cubic** and for the **Electric potential** dependent variable — **Linear**, **Quadratic** (the default), **Cubic**, or **Quartic**. For more information about the **Discretization** section, see [Settings for the Discretization Sections](#) in the *COMSOL Multiphysics Reference Manual*.



- [About the Magnetic and Electric Fields Interface Boundary Conditions](#)
- [Domain, Boundary, Edge, Point, and Pair Nodes for the Magnetic and Electric Fields Interface](#)
- [Theory for the Magnetic and Electric Fields Interface](#)

About the Magnetic and Electric Fields Interface Boundary Conditions

The Magnetic and Electric Fields interface boundary conditions are applied in a two-step procedure. This is because only some combinations of electric and magnetic boundary conditions are physically relevant whereas others can lead to unphysical models that violate the current conservation law.



The basic steps for this are to add the magnetic boundary conditions from the **Physics** toolbar. Then right-click these magnetic boundary condition nodes to add compatible electric boundary conditions as subnodes.

STEP 1: MAGNETIC BOUNDARY CONDITIONS

With no surface currents present the physics interface conditions

$$\mathbf{n}_2 \times (\mathbf{A}_1 - \mathbf{A}_2) = \mathbf{0}$$

$$\mathbf{n}_2 \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{0}$$

need to be fulfilled. Because the physics interface solves for \mathbf{A} , the tangential component of the magnetic potential is always continuous, and thus the first condition is automatically fulfilled. The second condition is equivalent to the natural boundary condition and is hence also fulfilled unless surface currents are explicitly introduced.

STEP 2: ELECTRIC BOUNDARY CONDITIONS

Depending on specific modeling problems, different electric boundary conditions should be used. To include the modeling of the full-wave effect, for instance, in the frequency domain studies, the most general exterior electric boundary condition is the **Ground**; that is,

$$V = 0$$

In some other cases where conducting current is more significant, other electric boundary conditions can be used. For example, at exterior boundaries between conducting and nonconducting materials, the general boundary condition is the **Electric Insulation**, expressed as

$$\mathbf{n} \cdot \mathbf{J} = 0$$

which is a natural boundary condition.



A default **Ground** subnode is also added under the default **Magnetic Insulation** node. This is to ensure that default boundary conditions are always specified both for the magnetic vector potential and the electric potential. Additional subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

Table 4-2 lists the interior and exterior boundary conditions available with this physics interface.

TABLE 4-2: INTERIOR AND EXTERIOR ELECTRIC AND MAGNETIC BOUNDARY CONDITIONS FOR THE MAGNETIC AND ELECTRIC FIELDS INTERFACE.

NODE	INTERIOR	EXTERIOR
MAGNETIC BOUNDARIES		
Background Magnetic Flux Density		x
Magnetic Continuity	x	
Magnetic Field		x
Magnetic Insulation	x	x
Magnetic Potential	x	x
Magnetic Shielding	x	
Perfect Magnetic Conductor	x	x
Surface Current	x	x
ELECTRIC BOUNDARIES		
Contact Impedance	x	
Electric Insulation	x	x
Electric Potential	x	x
Electric Shielding	x	
Floating Potential	x	x
Ground	x	x
Normal Current Density		x
Periodic Condition		x

BOUNDARY CONDITION COMBINATIONS

Table 4-3 shows the possible combination of magnetic and electric boundary conditions, with an explanation of the physical model represented by the more advanced combinations.

TABLE 4-3: POSSIBLE COMBINATIONS OF ELECTRIC AND MAGNETIC BOUNDARY CONDITIONS FOR THE MAGNETIC AND ELECTRIC FIELDS INTERFACE.

MAGNETIC FEATURE	ELECTRIC FEATURE	PHYSICAL MODEL
Magnetic Insulation	Electric Insulation	
	Electric Potential	
	Ground	
	Floating Potential	
	Terminal	
	Normal Current Density	
Magnetic Continuity	<none>	<no effect>
	Electric Insulation	Thin nonconducting, nonmagnetic layer, such as an air gap or crack in a metal. It can be used to model internal insulation.
	Contact Impedance	Thin resistive, nonmagnetic layer, such as an oxide layer in a metal.
Magnetic Shielding	<none>	Magnetic (high- μ_r) layer with same conductive properties as the surrounding medium.
	Electric Shielding	Thin magnetic, highly conductive layer (high- μ_r , high- σ).
	Electric Insulation	Thin nonconducting magnetic layer.
	Contact Impedance	Thin resistive magnetic layer.
Surface Current	<none>	Externally imposed surface current density.
	Electric Shielding	Thin nonmagnetic, highly conductive layer along which a surface current density flows, that is automatically included in the parent node.
Background Magnetic Flux Density	Electric Insulation	
	Electric Potential	
	Ground	

TABLE 4-3: POSSIBLE COMBINATIONS OF ELECTRIC AND MAGNETIC BOUNDARY CONDITIONS FOR THE MAGNETIC AND ELECTRIC FIELDS INTERFACE.

MAGNETIC FEATURE	ELECTRIC FEATURE	PHYSICAL MODEL
	Floating Potential	
	Terminal	
	Normal Current Density	

Domain, Boundary, Edge, Point, and Pair Nodes for the Magnetic and Electric Fields Interface

The [Magnetic and Electric Fields Interface](#) has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

Also see [About the Magnetic and Electric Fields Interface Boundary Conditions](#) and [Table 4-2](#) for a list of interior and exterior boundary conditions.



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

These nodes are described in this section:

- [Free Space](#)
- [Ampère’s Law and Current Conservation](#)
- [Background Magnetic Flux Density](#)
- [Initial Values](#)
- [Magnetic Continuity](#)
- [Magnetic Insulation](#)
- [Magnetic Shielding](#)
- [Surface Current](#)

The following nodes are described for the Magnetic Fields or Electric Currents interfaces,

- [Ampère’s Law](#)
- [Override Coil Inlet/Outlet](#)
- [Contact Impedance](#)
- [Edge Current](#)
- [Electric Insulation](#)
- [Electric Point Dipole](#)
- [Electric Point Dipole \(on Axis\)](#)
- [Electric Potential](#)
- [Electric Shielding](#)
- [External Current Density](#)
- [Floating Potential](#)
- [Gauge Fixing for A-Field](#)
- [Ground](#)
- [Magnetic Field](#)
- [Magnetic Point Dipole](#)
- [Magnetic Potential](#)
- [Normal Current Density](#)
- [Perfect Magnetic Conductor](#)
- [Terminal](#)



- [Sector Symmetry](#)
- [Infinite Elements, Perfectly Matched Layers, and Absorbing Layers in the COMSOL Multiphysics Reference Manual](#)



In the *COMSOL Multiphysics Reference Manual* see [Table 2-4](#) for links to common sections and [Table 2-5](#) to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Free Space

For inductive and capacitive (sometimes resistive) analysis, it is quite common for the fields to extend into the environment of the device in question. It is therefore important not only to model the device itself, but also its (close) surroundings. Typically, this is done by adding a box or sphere around the device’s geometry.

The default **Free Space** node is used to specify the physical conditions in close proximity to the device — *typically in air or vacuum*. It adds the Ampère’s law and current conservation *governing equations* with a limited set of material models: the permeability μ_r and permittivity ϵ_r are assumed to be one, and the conductivity is taken from the **Stabilization conductivity**.

The Free Space feature provides a canvas on top of which other features can be added to locally specify material properties and excitation forms.

STABILIZATION

Stabilization Conductivity

The **Stabilization conductivity** allows for four options:




- **From material**; use the conductivity specified by the material.
- **Automatic** (default); sets a conductivity $\sigma_{\text{stab}} = 1 \text{ S/m}$ for stationary and time dependent studies, and $\sigma_{\text{stab}} = 0$ otherwise. This is done in order to avoid getting a singular problem, which can happen when the conductivity is zero. For more information, see [Theory for the Magnetic and Electric Fields Interface](#).
- **Off**; disable the stabilization conductivity altogether: $\sigma_{\text{stab}} = 0$. This models a perfect vacuum and is a good approximation for air.
- **User defined**; specify a suitable stabilization conductivity directly.

Ampère’s Law and Current Conservation

The **Ampère’s Law and Current Conservation** node adds Ampère’s law and the equation of continuity for the electric current. It provides an interface for defining the constitutive relations and their associated properties. There are two types of this feature available, **Ampère’s Law and Current Conservation in Solids** and **Ampère’s Law and Current Conservation in Fluids**. This distinction decides how materials behave and how material properties are interpreted when the mesh is deformed.

Ampère’s Law and Current Conservation in Solids applies to materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame).

Ampère’s Law and Current Conservation in Fluids applies to materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined.

	<p>In COMSOL versions 6.2 and earlier, this Solids/Fluids distinction was controlled within the Ampère’s Law and Current Conservation node by specifying Solid/Nonsolid in the Material type setting.</p>
	<p>These features can be overridden with an Ampère’s Law feature or a Coil feature, which are identical to the ones in the Magnetic Fields interface, removing the electric potential and the current conservation equation from the selected domains.</p>
	<p>The Constitutive Relation Jc-E and Constitutive Relation B-H settings are the same as Ampère’s Law for the Magnetic Fields interface. The Constitutive Relation D-E settings are the same as for Current Conservation for the Electric Currents interface.</p>

Initial Values

The **Initial Values** node adds an initial value for the magnetic vector potential and electric potential that can serve as an initial value for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Magnetic vector potential \mathbf{A}** (SI unit: Wb/m) and initial value of the **Electric potential V** (SI unit: V). The default values are 0 Wb/m and 0 V, respectively.

Magnetic Insulation

The **Magnetic Insulation** node is the default magnetic boundary condition for the Magnetic and Electric Fields interface and sets the tangential components of the magnetic potential to zero at the boundary $\mathbf{n} \times \mathbf{A} = 0$. Electric boundary conditions can be applied by adding subnodes to the **Magnetic Insulation** node. The default electric boundary condition, added under each **Magnetic Insulation** node, is **Ground**. The **Electric Potential**, **Electric Insulation**, **Floating Potential**, **Terminal**, or **Normal Current**

Density subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.



About the Magnetic and Electric Fields Interface Boundary Conditions

Surface Current

The **Surface Current** node adds a boundary condition for a surface current density \mathbf{J}_s .

An externally applied surface current density can be specified directly in the **Settings** window for the node. Alternatively, the **Electric Shielding** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. Use the subnode to model a thin conductive layer (a layer whose electric conductivity s is higher than in the surrounding domains). In this case, the electric current flows preferably along the conductive boundary, and the resulting surface current density is automatically incorporated in the parent **Surface Current** node to act as a source for the magnetic field.

SURFACE CURRENT

Enter values or expressions for the **Surface current density** \mathbf{J}_{s0} (SI unit: A/m) coordinates.

Magnetic Shielding

The **Magnetic Shielding** node adds a boundary condition for magnetic shielding. By itself, this feature represents a geometrically thin layer with a relative permeability substantially higher than the surrounding material, that shields the magnetic field.

Subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. Use the subnodes to provide an electrical model on top of the Shielding magnetic model. The available subnodes are [Electric Shielding](#), [Electric Insulation](#), [Contact Impedance](#), and [Electrical Contact](#) (in the *AC/DC Module User's Guide*). The possible combinations are:

- **Magnetic Shielding** with no subnode: this represents a highly magnetic layer with no special electrical properties.
- **Magnetic Shielding** and **Electric Shielding**: this combination represents a layer in which both the relative permeability μ_r and the electric conductivity σ are much higher

than in the adjacent domain. This layer shields the magnetic field and the current preferentially flows along it. The resulting surface current density is incorporated in the model as a source for the magnetic field.

- **Magnetic Shielding** and **Electric Insulation**: this combination represents a nonconductive magnetic layer. The layer shields the magnetic field and there is no current flowing through it. The electric potential is discontinuous across the boundary.
- **Magnetic Shielding** and **Contact Impedance** or **Electrical Contact**: this combination represents a resistive magnetic layer. The layer shields the magnetic field and the current flows preferably orthogonally to the layer. The electric potential is discontinuous across the boundary.

MAGNETIC SHIELDING

The default **Relative permeability** μ_r (dimensionless) uses values **From material**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter other values or expressions. For anisotropic material, the relative permeability is a tensor.

Enter a value or expression for the **Surface thickness** d_s (SI unit: m).

Magnetic Continuity

The **Magnetic Continuity** node does not apply any condition or constraint to the model. Its purpose is to allow the application of electrical boundary conditions by means of the subnodes **Electric Insulation**, **Contact Impedance**, and **Electrical Contact** (in the *AC/DC Module User's Guide*). The subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. Use this feature to model thin layer with particular electrical properties but with the same magnetic properties of the surrounding medium.

Background Magnetic Flux Density

The **Background Magnetic Flux Density** node adds a boundary condition for the magnetic vector potential:

$$\mathbf{n} \times \mathbf{A} = \mathbf{n} \times \mathbf{A}_b$$

where \mathbf{A}_b is defined to satisfy:

$$\nabla \times \mathbf{A}_b = \mathbf{B}_b$$


where \mathbf{B}_b is defined in the **Magnetic Flux Density** section.

As the equation suggests, the boundary condition only guarantees that the tangential components of \mathbf{A} and \mathbf{A}_b are equal. Their normal components might deviate depending on specific situations. The **Background Magnetic Flux Density** node is incompatible with the **Periodic Condition** node. If periodicity is required in a background field, use the **Magnetic Potential** node along with the **Periodic Condition** node, and ensure that appropriate values are set consistently.



MAGNETIC FLUX DENSITY

Enter a value or expression for the **Magnetic flux density** \mathbf{B}_b (SI unit: T) components.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

The Electrical Circuit Interface

The **Electrical Circuit (cir)** interface (), found under the **AC/DC** branch () when adding a physics interface, is used to model currents and voltages in circuits including voltage and current sources, resistors, capacitors, inductors, and semiconductor devices. Models created with the Electrical Circuit interface can include connections to distributed field models. The physics interface supports stationary, frequency-domain and time-domain modeling and solves Kirchhoff's conservation laws for the voltages, currents, and charges associated with the circuit elements.

When this physics interface is added, it adds a default **Ground Node** feature and associates that with node zero in the electrical circuit.



Circuit nodes are nodes in the electrical circuit (electrical nodes) and should not be confused with nodes in the Model Builder tree of the COMSOL Multiphysics software. Circuit node names are not restricted to numerical values but can contain alphanumeric characters.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `cir`.

RESISTANCE IN PARALLEL TO PN JUNCTIONS

For numerical stability, a large resistance is added automatically in parallel to the pn junctions in diodes and BJT devices. Enter a default value for the **Resistance in parallel to pn junctions** R_j (SI unit: Ω). The default value is $1 \cdot 10^{12} \Omega$.


CREATE UNIQUE NODES FOR NEW DEVICES

When this setting is selected (the default), newly added devices will be assigned unused node names. The devices will be disconnected from the rest of the circuit and the nodes should be updated to reflect the actual circuit connections. When this setting is

deselected, new devices will be connected to the lowest-numbered nodes starting from 0.

ELECTRICAL CIRCUIT TOOLBAR

The following nodes are available from the **Electrical Circuit** ribbon toolbar (Windows users), **Electrical Circuit** context menu (Mac or Linux users), or right-click to access the context menu (all users):




For step-by-step instructions and general documentation descriptions, this is the **Electrical Circuit** toolbar.

- [Ground Node](#)
 - [Voltmeter](#)
 - [Ampère Meter](#)
 - [Resistor](#)
 - [Capacitor](#)
 - [Inductor](#)
 - [Voltage Source](#)
 - [Current Source](#)
 - [Diode](#)
 - [Switch](#)
 - [Voltage-Controlled Voltage Source](#)¹
 - [Voltage-Controlled Current Source](#)¹
 - [Current-Controlled Voltage Source](#)¹
 - [Current-Controlled Current Source](#)¹
- [Subcircuit Definition](#)
 - [Subcircuit Instance](#)
 - [Mutual Inductance](#)
 - [Transformer](#)
 - [NPN BJT and PNP BJT](#)²
 - [n-Channel MOSFET and p-Channel MOSFET](#)²
 - [External I vs. U](#)³
 - [External U vs. I](#)³
 - [External I-Terminal](#)³
 - [SPICE Circuit Import](#)
 - [SPICE Circuit Export](#)

¹ Selected from the **Dependent Sources** submenu when you right-click main node.
² Selected from the **Transistors** submenu when you right-click main node.
³ Selected from the **External Couplings** submenu when you right-click main node.

Ground Node


The **Ground Node** () feature adds a ground node with the default node number zero to the electrical circuit. This is the default node in the Electrical Circuit interface. More

ground nodes can be added but those must have unique node numbers and are by default given higher node numbers.

GROUND CONNECTION

Set the **Node name** for the ground node in the circuit. The convention is to use 0 (zero) for the ground node. If adding more ground nodes, each must have a unique node name (number).


Voltmeter

The **Voltmeter** () feature connects a voltmeter (voltage measurement device) between two nodes in the electrical circuit. A voltmeter behaves electrically as an open circuit. The voltmeter node adds a Probe sampling the voltage across it.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

Ampère Meter

The **Ammeter** () feature connects an ammeter (current measurement device) between two nodes in the electrical circuit. An ammeter behaves electrically as a short circuit. The ammeter node adds a Probe sampling the current through it.


NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

DEVICE PARAMETERS

Enter the **Resistance** of the resistor.

Resistor

The **Resistor** () feature connects a resistor between two nodes in the electrical circuit.


NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the resistor.

DEVICE PARAMETERS

Enter the **Resistance** of the resistor.

Capacitor

The **Capacitor** () feature connects a capacitor between two nodes in the electrical circuit.


NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the capacitor.

DEVICE PARAMETERS

Enter the **Capacitance** of the capacitor.

Inductor

The **Inductor** () feature connects an inductor between two nodes in the electrical circuit.


NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the inductor.

DEVICE PARAMETERS

Enter the **Inductance** of the inductor.

Voltage Source

The **Voltage Source** () feature connects a voltage source between two nodes in the electrical circuit.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.

DEVICE PARAMETERS

Enter the **Source type** that should be adapted to the selected study type. It can be **General source**, **AC-source**, or a time-dependent **Sine source** or **Pulse source**. Depending on the choice of source, also specify the following parameters:

- For a General source, the **Voltage V_{src}** (default value: 1 V). General sources are active in Stationary, Time-Dependent and Frequency Domain studies.
- For an AC-source: the **Voltage V_{src}** (default value: 1 V) and the **Phase Θ** (default value: 0 rad). AC-sources are active in Frequency Domain studies only.


- For a sine source: the **Voltage V_{src}** (default value: 1 V), the **Offset V_{off}** (default value: 0 V), the **Frequency** (default value: 1 kHz), and the **Phase Θ** (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.
- For a pulse source: the **Voltage V_{src}** (default value: 1 V), the **Offset V_{off}** (default value: 0 V), the **Delay t_d** (default value: 0s), the **Rise time t_r** and **Fall time t_f** (default values: 0 s), the **Pulse width p_w** (default value: 1 μ s), and the **Period T_{per}** (default value: 2 μ s). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

All values are peak values rather than RMS.



For the AC source, the frequency is a global input set by the solver. AC sources should be used in Frequency-domain studies only. Do not use the **Sine source** unless the model is time dependent.

Current Source

The **Current Source** () feature connects a current source between two nodes in the electrical circuit.

NODE CONNECTIONS

Set the two **Node names** for the connecting nodes for the current source. The first node represents the positive reference terminal from where the current flows through the source to the second node.

DEVICE PARAMETERS

Enter the **Source type** that should be adapted to the selected study type. It can be **General source**, **AC-source**, or a time-dependent **Sine source** or **Pulse source**. Depending on the choice of source, also specify the following parameters:

- For a General source, the **Current i_{src}** (default value: 1 A). General sources are active in Stationary, Time-Dependent and Frequency Domain studies.
- For an AC-source: the **Current i_{src}** (default value: 1 A) and the **Phase Θ** (default value: 0 rad). AC-sources are active in Frequency Domain studies only.


- For a sine source: the **Current** i_{src} (default value: 1 A), the **Offset** i_{off} (default value: 0 A), the **Frequency** (default value: 1 kHz), and the **Phase** Θ (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.
- For a pulse source: the **Current** i_{src} (default value: 1 A), the **Offset** i_{off} (default value: 0 A), the **Delay** t_d (default value: 0 s), the **Rise time** t_r and **Fall time** t_f (default values: 0 s), the **Pulse width** p_w (default value: 1 μ s), and the **Period** T_{per} (default value: 2 μ s). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for t has been provided as a model parameter or global variable.

All values are peak values rather than RMS.



For the AC source, the frequency is a global input set by the solver. AC sources should be used in frequency-domain studies only. Do not use the **Sine source** unless the model is time dependent.

Voltage-Controlled Voltage Source

The **Voltage-Controlled Voltage Source** () feature connects a voltage-controlled voltage source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.


NODE CONNECTIONS

Specify four **Node names**: the first pair for the connection nodes for the voltage source and the second pair defining the input control voltage. The first node in a pair represents the positive reference terminal.

DEVICE PARAMETERS

There are two options to define the relationship between the control voltage and resulting voltage. The **Use gain** method defines the resulting voltage to be the control voltage multiplied by the gain. The **Custom expression** method can define the relationship with an arbitrary expression.

Voltage-Controlled Current Source

The **Voltage-Controlled Current Source** () feature connects a voltage-controlled current source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.


NODE CONNECTIONS

Specify four **Node names**: the first pair for the connection nodes for the current source and the second pair defining the input control voltage. The first node in a pair represents the positive voltage reference terminal or the one from where the current flows through the source to the second node.

DEVICE PARAMETERS

There are two options to define the relationship between the control voltage and resulting current. The **Use gain** method defines the resulting current to be the control voltage multiplied by the gain (SI units: S). The **Custom expression** method can define the relationship with an arbitrary expression.

Current-Controlled Voltage Source

The **Current-Controlled Voltage Source** () feature connects a current-controlled voltage source between two nodes in the electrical circuit. The input control current is the one flowing through a two-pin device.


NODE CONNECTIONS

Set two **Node names** for the connection nodes for the voltage source. The first node in a pair represents the positive reference terminal.

DEVICE PARAMETERS

There are two options to define the relationship between the control current and resulting voltage. The **Use gain** method defines the resulting voltage to be the control current multiplied by the gain (SI units: Ω). The **Custom expression** method can define the relationship with an arbitrary expression.

Current-Controlled Current Source

The **Current-Controlled Current Source** () feature connects a current-controlled current source between two nodes in the electrical circuit. The input control current is the one flowing through a named device that must be a two-pin device.


NODE CONNECTIONS

Specify two **Node names** for the connection nodes for the current source. The first node in a pair represents the positive reference terminal from where the current flows through the source to the second node.

DEVICE PARAMETERS

There are two options to define the relationship between the control current and resulting current. The **Use gain** method defines the resulting current to be the control current multiplied by the gain. The **Custom expression** method can define the relationship with an arbitrary expression.

Switch

The **Switch** () feature is used to connect or disconnect the conducting path in a circuit under specific conditions.

NODE CONNECTIONS

Specify two **Node names** for the connection nodes for the current source. The first node in a pair represents the positive reference terminal from where the current flows through the source to the second node.

SWITCH CONDITIONS

There are three types of conditions, **Voltage controlled**, **Current controlled**, and **Custom expressions**. For each type of condition there are two conditions, one for turn on and one for turn off. The on condition is true if the **On condition** expression is larger than zero, while the off condition is true if the **Off condition** is less than zero.

Note: The state of the switch (on/off) is changed only when a condition goes from false to true and not when going from true to false. Thus, if the state is off and the on condition goes from false to true, the state will shift from off to on. On the other hand, if the state of the switch is on and the on condition goes from true to false, nothing will happen.

The **Initial state** list has three options, **Use on condition**, **Use off condition**, and **Boolean expression**. The two former options mean that the switch will have an initial state matching to the on or off condition. The third option makes the switch's initial state


match a custom Boolean expression. Separating on, off, and initial states makes the switch more flexible and can support Schmitt-trigger style switches and various latches.

For the **Voltage controlled** switch, it is necessary to specify two nodes that defines the voltage `sens.v` that the switch state depends on. The conditions must be written as a function of this variable. Similarly, for the **Current controlled** switch it is necessary to specify a two-pin device that defines the current `sens.i` that the switch state depends on.

SWITCH PARAMETERS

When the switch is in the on state it has a nonzero resistance specified by the **On resistance** expression. For the off state no current flows through the switch (infinite resistance). There is also a transition time for the switch to turn on and off set by the **Switching time** expression. The switch triggers an implicit event that updates a discrete state variable (with suffix `_state`).


Subcircuit Definition

The **Subcircuit Definition** () feature is used to define subcircuits, which can be inserted as devices into the main circuit using **Subcircuit Instance** nodes. Create the subcircuit by adding subnodes to the **Subcircuit Definition** node, either by using the **Physics** toolbar, or by right-clicking the **Subcircuit Definition**.


SUBCIRCUIT PINS

Define the **Pin names** at which the subcircuit connects to the main circuit or to other subcircuits when referenced by a **Subcircuit Instance** node. The **Pin names** refer to circuit nodes in the subcircuit. The order in which the **Pin names** are defined is the order in which they are referenced by a Subcircuit Instance node. The devices constituting the subcircuit should be connected only to the subcircuit's pins and to themselves.

INPUT PARAMETERS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options**. Specify input parameters to a subcircuit that can be changed from a subcircuit instance. These input parameters can be used in all expression-style edit fields that affect the parameters of a device, for example, resistance, capacitance, and current gain. In this way, a subcircuit can represent a parameterized custom device model.


Subcircuit Instance

The **Subcircuit Instance** () feature represents an instance of a subcircuits defined by a [Subcircuit Definition](#) feature.



NODE CONNECTIONS

Select the **Name of subcircuit link** from the list of defined subcircuits in the circuit model and the circuit **Node names** at which the subcircuit instance connects to the main circuit or to another subcircuit if used therein.

INPUT PARAMETERS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options**. Specify input parameters to a subcircuit that can be changed from a subcircuit instance. These input parameters can be used in all expression-style edit fields that affect the parameters of a device, for example, resistance, capacitance, and current gain. In this way, a subcircuit can represent a parameterized custom device model.

NPN BJT and PNP BJT

The **NPN BJT** () and the **PNP BJT** () device models are large-signal models for bipolar junction transistors (BJT). It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model input parameters for this BJT model. For any particular make of BJT, the device manufacturer should be the primary source of information.

NODE CONNECTIONS

Specify three **Node names** for the connection nodes for the **BJT** device. These represent the *collector*, *base*, and *emitter* nodes for the **NPN** transistor, and the *emitter*, *base*, and *collector* nodes for the **PNP** transistor.

MODEL PARAMETERS



Specify the **Model Parameters**. Reasonable defaults are provided but for any particular BJT, the device manufacturer should be the primary source of information.



The interested reader is referred to [Ref. 1](#) for more details on semiconductor modeling within circuits.

For an explanation of the **Model Parameters** see [BJT Transistors](#).

n-Channel MOSFET and p-Channel MOSFET

The **n-Channel MOSFET** () and the **p-Channel MOSFET** () device models are large-signal models for, respectively, an n-Channel MOS field-effect transistor (MOSFET) and p-Channel MOSFET. These are advanced device models and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model parameters for the MOSFET models. For any particular make of MOSFET, the device manufacturer should be the primary source of information.

NODE CONNECTIONS

Specify four **Node names** for the connection nodes for the **n-Channel MOSFET** or **p-Channel MOSFET** device. These represent the *drain*, *gate*, *source*, and *bulk* nodes, respectively.

MODEL PARAMETERS

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular MOSFET, the device manufacturer should be the primary source of information.



The interested reader is referred to [Ref. 1](#) for more details on semiconductor modeling within circuits.

For an explanation of the **Model Parameters** see [MOSFET Transistors](#).

Mutual Inductance

The **Mutual Inductance** allows specifying a coupling between two existing [Inductor](#) features in the circuit. The mutual inductance of the coupling is

$$M = k\sqrt{L_1 L_2}$$

where k is the coupling factor and L_1 and L_2 are the inductances of the inductors.

DEVICE PARAMETERS

Enter values or expressions for the:

- **Coupling factor** k (dimensionless). The value must be between 0 and 1, and the default is 0.98.
- **First inductance** L_1 (SI unit: H) and **Second inductance** L_2 (SI unit: H). These must be set to two different [Inductor](#) features in the circuit.

Transformer

The **Transformer** feature represents either a combination of two [Inductor](#) and a [Mutual Inductance](#) features, or an ideal transformer.

NODE CONNECTIONS

Enter or edit the table in the **Node names** column for the **primary** and **secondary** node connections.

DEVICE PARAMETERS


Choose a **Transformer model** — **Specify inductors** (the default) or **Ideal transformer**.

For **Specify inductors** enter values or expressions for the:

- **Coupling factor** k (dimensionless). The default is 0.98.
- **First inductance** L_1 (SI unit: H). The default is 1 mH.
- **Second inductance** L_2 (SI unit: H). The default is 1 mH.

For **Ideal transformer** enter values or expressions for the **Winding ratio** N_1/N_2 (dimensionless). The default is 10.

Diode

The **Diode** device model () is a large-signal model for a diode. It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. The interested reader is referred to [Ref. 1](#) for more details on semiconductor modeling within circuits. Many device manufacturers

provide model parameters for this diode model. For any particular make of diode, the device manufacturer should be the primary source of information.

NODE CONNECTIONS

Specify two **Node names** for the positive and negative nodes for the **Diode** device.


MODEL PARAMETERS

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular diode, the device manufacturer should be the primary source of information.



For an explanation of the **Model Parameters** see [Diode](#).

External I vs. U

The **External I vs. U** () feature connects an arbitrary voltage measurement (for example, a circuit terminal or circuit port boundary or a coil domain from another physics interface) as a voltage source between two nodes in the electrical circuit. The resulting circuit current from the first node to the second node is typically coupled back as a prescribed current source in the context of the voltage measurement.



NODE CONNECTIONS

Specify the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.


EXTERNAL DEVICE

Enter the source of the **Voltage**. If circuit or current excited terminals or circuit ports are defined on boundaries or domains or a multiturn coil domains is defined in other physics interfaces, these display as options in the **Voltage** list. Also select the **User defined** option and enter your own voltage variable, for example, using a suitable coupling operator. For inductive or electromagnetic wave propagation models, the voltage measurement must be performed as an integral of the electric field because the electric

potential only does not capture induced EMF. Also the integration must be performed over a distance that is short compared to the local wavelength.

	Except when coupling to a circuit terminal, circuit port, or coil, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention <code>cirn.IvsUm_i</code> , where <code>cirn</code> is the tag of the Electrical Circuit interface node and <code>IvsUm</code> is the tag of the External I vs. U node. The tags are typically displayed within curly brackets <code>{ }</code> in the Model Builder.
	Nonlocal Couplings and Coupling Operators in the <i>COMSOL Multiphysics Reference Manual</i>

External U vs. I

The **External U vs. I** () feature connects an arbitrary current measurement (for example, a coil domain from another physics interface) as a current source between two nodes in the electrical circuit. The resulting circuit voltage between the first node and the second node is typically coupled back as a prescribed voltage source in the context of the current measurement.



NODE CONNECTIONS

Specify the two **Node names** for the connecting nodes for the current source. The current flows from the first node to the second node.


EXTERNAL DEVICE

Enter the source of the **Current**. Voltage excited terminals or lumped ports defined on boundaries in other physics interfaces are natural candidates but do not appear as options in the **Voltage** list because those do not have an accurate built-in current

measurement variable. A **User defined** option must be selected and a current variable entered, for example, using a suitable coupling operator.

	The voltage variable must be manually coupled back in the electrical circuit to the context of the current measurement. This applies also when coupling to a voltage excited terminal or lumped port. The name of this voltage variable follows the convention <code>cirn.UvsIm_v</code> , where <code>cirn</code> is the tag of the Electrical Circuit interface node and <code>UvsIm</code> is the tag of the External U vs. I node. The tags are typically displayed within curly brackets {} in the Model Builder.
	Nonlocal Couplings and Coupling Operators in the <i>COMSOL Multiphysics Reference Manual</i>

External I-Terminal

The **External I-Terminal** () feature connects an arbitrary voltage-to-ground measurement (for example, a circuit terminal from another physics interface) as a voltage-to-ground assignment to a node in the electrical circuit. The resulting circuit current from the node is typically coupled back as a prescribed current source in the context of the voltage measurement. This node does not apply when coupling to inductive or electromagnetic wave propagation models because then voltage must be defined as a line integral between two points rather than a single point measurement of electric potential. For such couplings, use the [External I vs. U](#) node instead.



NODE CONNECTIONS

Set the **Node name** for the connecting node for the voltage assignment.


EXTERNAL TERMINAL


Enter the source of the **Voltage**. If circuit- or current-excited terminals are defined on boundaries in other physics interfaces, these display as options in the **Voltage** list. Also

select the **User defined** option and enter a voltage variable, for example, using a suitable coupling operator.


	<ul style="list-style-type: none">• Except when coupling to a circuit terminal, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention <code>cirn.termIm_i</code>, where <code>cirn</code> is the tag of the Electrical Circuit interface node and <code>termIm</code> is the tag of the External I-Terminal node. The tags are typically displayed within curly brackets <code>{ }</code> in the Model Builder.• When connecting the finite element model between two circuit nodes that both are not grounded, the External I-Terminal node cannot be used. In this case, use External I vs. U or External U vs. I instead.
	Nonlocal Couplings and Coupling Operators in the <i>COMSOL Multiphysics Reference Manual</i> .

SPICE Circuit Import

Right-click the **Electrical Circuit** () feature node to import an existing SPICE netlist (select **Import Spice Netlist**). A window opens — enter a file location or browse your directories to find one. The default file extension for a SPICE netlist is `.cir`. The SPICE circuit import translates the imported netlist into Electrical Circuit interface nodes so these define the subset of SPICE features that can be imported.

	See SPICE Import about the supported SPICE commands.
---	--

SPICE Circuit Export

Right-click the **Electrical Circuit** () feature node to export the current circuit to the SPICE netlist file format (select **Export Spice Netlist** ). A window opens — enter a

file location or browse your directories to find one. The default file extension for a SPICE netlist is `.cir`. The compatible circuit nodes are exported as SPICE devices



See [SPICE Export](#) for more details on the supported SPICE commands.

Theory for the Electrostatics Interface

The [Electrostatics Interface](#) is available for 3D, 2D in-plane, and 2D axisymmetric components. Applications with electrostatic equations include high-voltage apparatus, electronic devices, and capacitors. The term “statics” is not to be interpreted literally — it is the observation time, or time scale at which the applied excitation changes, that is short compared to the charge relaxation time; also, the electromagnetic wavelength and skin depth are very large compared to the size of the domain of interest.

If you do not know whether to use the Electric Currents or the Electrostatics interface, which both solve for the scalar electric potential V , consider using an explicit charge transport model. See [Charge Relaxation Theory](#).

Charge Relaxation Theory

COMSOL Multiphysics includes physics interfaces for the modeling of static electric fields and currents. Deciding what specific physics interface and study type to select for a particular modeling situation requires a basic understanding of the charge dynamics in conductors.

The different physics interfaces involving only the scalar electric potential can be interpreted in terms of the charge relaxation process. The fundamental equations involved are *Ohm's law* for the conduction current density

$$\mathbf{J}_c = \sigma \mathbf{E}$$

the *equation of continuity*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J}_c = 0$$

and *Gauss' law*

$$\nabla \cdot (\epsilon \mathbf{E}) = \rho$$

By combining these, one can deduce the following differential equation for the space charge density in a homogeneous medium

$$\frac{\partial \rho}{\partial t} + \frac{\sigma}{\epsilon} \rho = 0$$

This equation has the solution

$$\rho(t) = \rho_0 e^{-t/\tau}$$

where

$$\tau = \frac{\epsilon}{\sigma}$$

is called the charge relaxation time. For a good conductor like copper, τ is of the order of 10^{-19} s, whereas for a good insulator like silica glass, it is of the order of 10^3 s. For a pure insulator, it becomes infinite.

When modeling real-world devices, there is not only the *intrinsic time scale* of the charge relaxation time but also an *external time scale* t at which a device is energized or the observation time. It is the relation between the external time scale and the charge relaxation time that determines what physics interface and study type to use. The results are summarized in [Table 4-4](#) below,

TABLE 4-4: SUITABLE PHYSICS INTERFACE AND STUDY TYPE FOR DIFFERENT TIME-SCALE REGIMES.

CASE	PHYSICS INTERFACE	STUDY TYPE
$\tau \gg t$	Electrostatics	Stationary
$\tau \ll t$	Electric Currents	Stationary
$\tau \sim t$	Electric Currents	Time Dependent or Frequency Domain

FIRST CASE: $\tau \gg t$

If the external time scale is short compared to the charge relaxation time, the charges do not have time to redistribute to any significant degree. Thus the charge distribution can be considered as a given model input. The best approach is to solve the Electrostatics formulation using the electric potential V .

By combining the definition of the potential with Gauss' law, you can derive the classical Poisson's equation. Under static conditions, the electric potential V is defined by the equivalence $\mathbf{E} = -\nabla V$. Using this together with the constitutive relation $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$ between \mathbf{D} and \mathbf{E} , you can rewrite Gauss' law as a variant of Poisson's equation

$$-\nabla \cdot (\epsilon_0 \nabla V - \mathbf{P}) = \rho$$

This equation is used in the Electrostatics interface. It is worth noting that Gauss' law does not require the charge distribution to be static. Thus, provided dynamics are slow enough that induced electric fields can be neglected and hence a scalar electric potential is justified, the formulation can be used also in the Time Dependent study type. That typically involves either prescribing the charge dynamics or coupling a separate formulation for this.



Such separate charge transport formulations can be found in the Electric Discharge Module, the Plasma Module, the Semiconductor Module, and the Chemical Reaction Engineering Module.

SECOND CASE: $\tau \ll T$

If the external time scale is long compared to the charge relaxation time, the stationary solution to the equation of continuity has been reached. In a stationary coordinate system, a slightly more general form of Ohm's law than above states that

$$\mathbf{J}_c = \sigma \mathbf{E} + \mathbf{J}_e$$

where \mathbf{J}_e is an externally generated current density. The static form of the equation of continuity then reads

$$\nabla \cdot \mathbf{J}_c = -\nabla \cdot (\sigma \nabla V - \mathbf{J}_e) = 0$$

To handle current sources, the equation can be generalized to

$$-\nabla \cdot (\sigma \nabla V - \mathbf{J}_e) = Q_j$$

This equation is used in the static study type for the Electric Currents interface.

GENERAL CASE: CHARGE DYNAMICS

If the charge relaxation time is comparable to the external time scale, the Time Dependent or Frequency Domain study types for the Electric Currents interface must be used.

Combining the time-harmonic equation of continuity

$$\nabla \cdot \mathbf{J}_c = \nabla \cdot (\sigma \mathbf{E} + \mathbf{J}_e) = -j\omega \rho$$

with the equation $(\nabla \cdot \mathbf{D} = \rho)$ yields the following equation for the frequency domain study type:

$$-\nabla \cdot ((\sigma + j\omega\epsilon_0)\nabla V - (\mathbf{J}_e + j\omega\mathbf{P})) = 0$$

For the Time Dependent study type, use the transient equation of continuity

$$\nabla \cdot \mathbf{J}_e = \nabla \cdot (\sigma\mathbf{E} + \mathbf{J}_e) = -\frac{\partial \rho}{\partial t}$$

and the resulting equation becomes

$$-\nabla \cdot \frac{\partial}{\partial t}(\epsilon_0\nabla V + \mathbf{P}) - \nabla \cdot (\sigma\nabla V - \mathbf{J}_e) = 0$$

These dynamic formulations are valid as long as induced electric fields can be ignored and hence the electric field is essentially curl free. This condition is fulfilled provided that skin effect and wave propagation effects can be ignored. The skin depth must be much larger than the geometrical dimensions of the modeled device and so must the wavelength. Note also that these formulations can be used to model dielectric regions of capacitive/resistive devices even though the interior of electrodes sometimes does not meet the large skin depth condition. In that case, the electrodes must only be represented as boundary conditions (fixed or floating potential). The interior, metallic domains are not included in the analysis. Obviously, this is only a valid approach for devices where metallic electrodes do not entirely bypass (short circuit) the capacitive/resistive layers. If metallic electrodes short circuit the capacitive/resistive layers, the time evolution of the current is determined by inductive and resistive effects with very little influence from the capacitive layers. Then the Magnetic Fields interface is the appropriate modeling tool.

Electrostatics Equations

Under static conditions, the electric potential, V , is defined by the relationship:

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

Combining this equation with the constitutive relationship $\mathbf{D} = \epsilon_0\mathbf{E} + \mathbf{P}$ between the electric displacement \mathbf{D} and the electric field \mathbf{E} , it is possible to represent Gauss' law as the following equation:

$$-\nabla \cdot (\epsilon_0\nabla V - \mathbf{P}) = \rho$$

In this equation, the physical constant, ϵ_0 (SI unit: F/m) is the permittivity of vacuum, \mathbf{P} (SI unit: C/m²) is the electric polarization vector, and ρ (SI unit: C/m³) is a space charge density. This equation describes the electrostatic field in dielectric materials.

For in-plane 2D modeling, the Electrostatics interface assumes a symmetry where the electric potential varies only in the x and y directions and is constant in the z direction. This implies that the electric field, \mathbf{E} , is tangential to the xy -plane. With this symmetry, the same equation is solved as in the 3D case. The physics interface solves the following equation where d is the thickness in the z direction:

$$-\nabla \cdot d(\epsilon_0 \nabla V - \mathbf{P}) = \rho$$

The axisymmetric version of the physics interface considers the situation where the fields and geometry are axially symmetric. In this case, the electric potential is constant in the ϕ direction, which implies that the electric field is tangential to the rz -plane.

The Electrostatics Interface in Time Dependent or Frequency Domain Studies

The [Electrostatics Interface](#) can also be solved in a dynamic study (Time Dependent or Frequency Domain). The equation system solved, however, is typically always the one presented in the previous section for the stationary case, in which no transient electromagnetic effects are taken into account. The difference is that the sources of the problem (charge densities, electric potential) are assumed to be time-varying (in a Time Dependent study) or time-harmonic (in a Frequency Domain study).

The support for dynamic studies simplifies the coupling of the Electrostatics interface with other physics interfaces. Using the physics interface in a dynamic study is a valid approximation only if the time-scale (or the frequency) of the study is so slow that transient electromagnetic effects can be neglected; for example, in acoustic or structural problems.

Most of the features in the Electrostatics interface have the same behavior in all study types, with the important exception of the Terminal node.

The Electrostatics interface also supports the small-signal analysis study sequence, which can be used when a time-harmonic perturbation is superposed on a static bias charge or voltage.

Theory for the Magnetic and Electric Fields Interface

The [Magnetic and Electric Fields Interface](#) can be used for modeling full coupling between electric and magnetic fields. Use this physics interface for 3D, 2D, and 2D axisymmetric components. For a deeper theoretical background to the magnetic vector potential and electric scalar potential used below, see the [Theory for the Magnetic Fields Interface](#).

In this section:

- [Stationary Equations](#)
- [Time Domain Equations](#)

Stationary Equations

To derive the stationary equations, start with Ampère's law for static cases: $\nabla \times \mathbf{H} = \mathbf{J}$. Define the potentials,

$$\begin{aligned}\mathbf{B} &= \nabla \times \mathbf{A} \\ \mathbf{E} &= -\nabla V\end{aligned}$$

and the current

$$\mathbf{J} = \sigma \mathbf{v} \times \mathbf{B} - \sigma \nabla V + \mathbf{J}_e$$

where \mathbf{J}_e is an externally generated current density, and \mathbf{v} is the velocity of the conductor.

Add the constitutive relationship, $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$, and rewrite Ampère's law as

$$\nabla \times (\mu_0^{-1} \nabla \times \mathbf{A} - \mathbf{M}) - \sigma \mathbf{v} \times (\nabla \times \mathbf{A}) + \sigma \nabla V = \mathbf{J}_e$$

The equation of continuity is obtained by taking the divergence of Ampère's law. It is the equation solved for the electric potential. Thus the following equations for V and \mathbf{A} apply:

$$\begin{aligned}-\nabla \cdot (-\sigma \mathbf{v} \times (\nabla \times \mathbf{A}) + \sigma \nabla V - \mathbf{J}_e) &= 0 \\ \nabla \times (\mu_0^{-1} \nabla \times \mathbf{A} - \mathbf{M}) - \sigma \mathbf{v} \times (\nabla \times \mathbf{A}) + \sigma \nabla V &= \mathbf{J}_e\end{aligned}$$

Time Domain Equations

The time domain equations are based on [Maxwell's Equations \(Quasistatic\)](#). The time domain formulation is the same as the [Stationary Equations](#), except that the electric field is defined as

$$\mathbf{E} = -\nabla V - \frac{\partial \mathbf{A}}{\partial t}$$

The time domain formulation is inherently ungauged, see [Gauge Transformations](#).

Theory for the Electrical Circuit Interface

The [Electrical Circuit Interface](#) theory is discussed in this section:

- [Electrical Circuit Modeling and the Semiconductor Device Models](#)
- [Bipolar Transistors](#)
- [MOSFET Transistors](#)
- [Diode](#)
- [Reference for the Electrical Circuit Interface](#)



Electrical Circuit Modeling and the Semiconductor Device Models

Electrical circuit modeling capabilities are useful when simulating all sorts of electrical and electromechanical devices ranging from heaters and motors to advanced plasma reactors in the semiconductor industry. There are two fundamental ways that an electrical circuit model relates to a physical field model.

- The field model is used to get a better, more accurate description of a single device in the electrical circuit model.
- The electrical circuit is used to drive or terminate the device in the field model in such a way that it makes more sense to simulate both as a tightly coupled system.

The Electrical Circuit interface makes it possible to add nodes representing circuit elements directly to the Model Builder tree in a COMSOL Multiphysics model. The circuit variables can then be connected to a physical device model to perform co-simulations of circuits and multiphysics. The model acts as a device connected to the circuit so that its behavior is analyzed in larger systems.

The fundamental equations solved by the Electrical Circuit interface are Kirchhoff's circuit laws, which in turn can be deduced from Maxwell's equations. The supported study types are Stationary, Frequency Domain, and Time Dependent.

There are three more advanced large-signal semiconductor device features available in the Electrical Circuit interface. The equivalent circuits and the equations defining their nonideal circuit elements are described in this section. For a more complete treatise on semiconductor device modeling, see [Ref. 1](#).

Bipolar Transistors

[Figure 4-1](#) illustrates the equivalent circuit for the npn bipolar junction transistor.

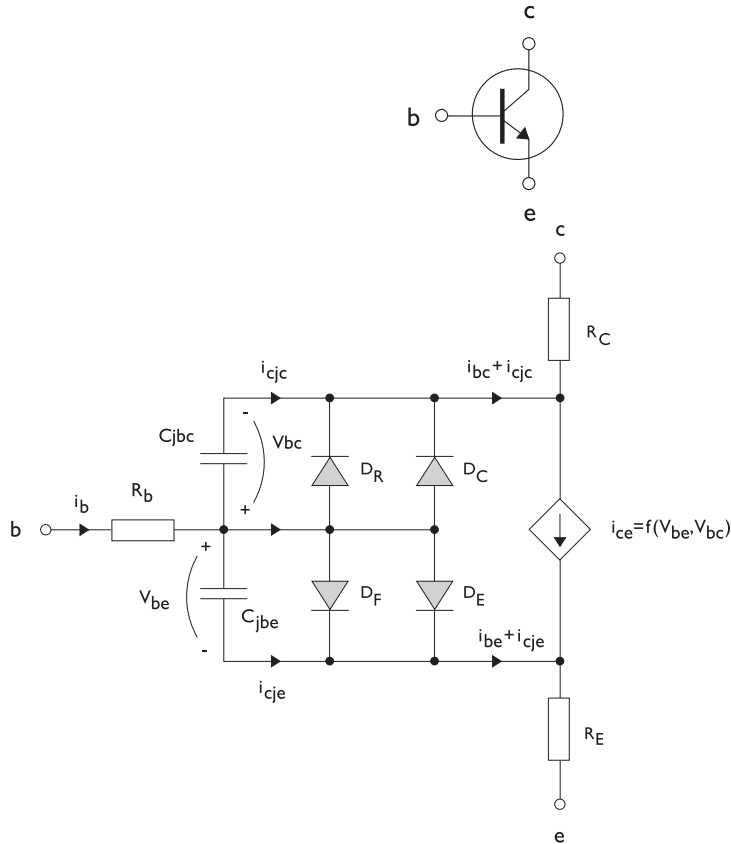


Figure 4-1: A circuit for the bipolar transistor.

The pnp transistor model is similar in all regards to the npn transistor, with the difference that the polarities of the currents and voltages involved are reversed. The following equations are used to compute the relations between currents and voltages in the circuit.

$$v_{rb} = \frac{1}{A} \left(R_{BM} - \frac{R_B - R_{BM}}{f_{bq}} \right) i_b$$

$$f_{bq} = \frac{1}{2 \left(1 - \frac{v_{bc}}{V_{AF}} - \frac{v_{be}}{V_{AR}} \right)} \left(1 + \sqrt{1 + 4 I_S \left(\frac{e^{\frac{v_{be}}{N_F V_T}} - 1}{I_{KF} A} + \frac{e^{\frac{v_{bc}}{N_R V_T}} - 1}{I_{KR} A} \right)} \right)$$

$$i_{be} = A \left(\frac{I_S}{B_F} \left(e^{\frac{v_{be}}{N_F V_T}} - 1 \right) + I_{SE} \left(e^{\frac{v_{be}}{N_E V_T}} - 1 \right) \right)$$

$$i_{bc} = A \left(\frac{I_S}{B_R} \left(e^{\frac{v_{bc}}{N_R V_T}} - 1 \right) + I_{SC} \left(e^{\frac{v_{bc}}{N_C V_T}} - 1 \right) \right)$$

$$i_{ce} = A \left(\frac{I_S}{f_{bq}} \left(e^{\frac{v_{be}}{N_F V_T}} + e^{\frac{v_{bc}}{N_C V_T}} \right) \right)$$

$$V_T = \frac{k_B T_{NOM}}{q}$$

There are also two capacitances that use the same formula as the junction capacitance of the diode model. In the parameter names below, replace x with C for the base-collector capacitance and E for the base-emitter capacitance.

$$C_{jbx} = AC_{Jx} \times \begin{cases} \left(1 - \frac{v_{bx}}{V_{Jx}} \right)^{-M_{Jx}} & v_{bx} < F_C V_{Jx} \\ (1 - F_C)^{-1 - M_{Jx}} \left(1 - F_C (1 + M_{Jx}) + M_{Jx} \frac{v_{bx}}{V_{Jx}} \right) & v_{bx} \geq F_C V_{Jx} \end{cases}$$

The model parameters are listed in the table below.

TABLE 4-1: BIPOLAR TRANSISTOR MODEL PARAMETERS.

PARAMETER	DEFAULT	DESCRIPTION
B_F	100	Ideal forward current gain
B_R	1	Ideal reverse current gain
C_{JC}	0 F/m ²	Base-collector zero-bias depletion capacitance
C_{JE}	0 F/m ²	Base-emitter zero-bias depletion capacitance
F_C	0.5	Breakdown current
I_{KF}	Inf (A/m ²)	Corner for forward high-current roll-off
I_{KR}	Inf (A/m ²)	Corner for reverse high-current roll-off

TABLE 4-1: BIPOLAR TRANSISTOR MODEL PARAMETERS.

PARAMETER	DEFAULT	DESCRIPTION
I_S	10^{-15} A/m^2	Saturation current
I_{SC}	0 A/m^2	Base-collector leakage saturation current
I_{SE}	0 A/m^2	Base-emitter leakage saturation current
M_{JC}	1/3	Base-collector grading coefficient
M_{JE}	1/3	Base-emitter grading coefficient
N_C	2	Base-collector ideality factor
N_E	1.4	Base-emitter ideality factor
N_F	1	Forward ideality factor
N_R	1	Reverse ideality factor
R_B	$0 \text{ } \Omega \cdot \text{m}^2$	Base resistance
R_{BM}	$0 \text{ } \Omega \cdot \text{m}^2$	Minimum base resistance
R_C	$0 \text{ } \Omega \cdot \text{m}^2$	Collector resistance
R_E	$0 \text{ } \Omega \cdot \text{m}^2$	Emitter resistance
T_{NOM}	298.15 K	Device temperature
V_{AF}	Inf (V)	Forward Early voltage
V_{AR}	Inf (V)	Reverse Early voltage
V_{JC}	0.71 V	Base-collector built-in potential
V_{JE}	0.71 V	Base-emitter built-in potential

Figure 4-2 illustrates an equivalent circuit for the n-channel MOSFET transistor. The p-channel MOSFET transistor is treated similarly, but the polarities of the involved voltages are reversed.

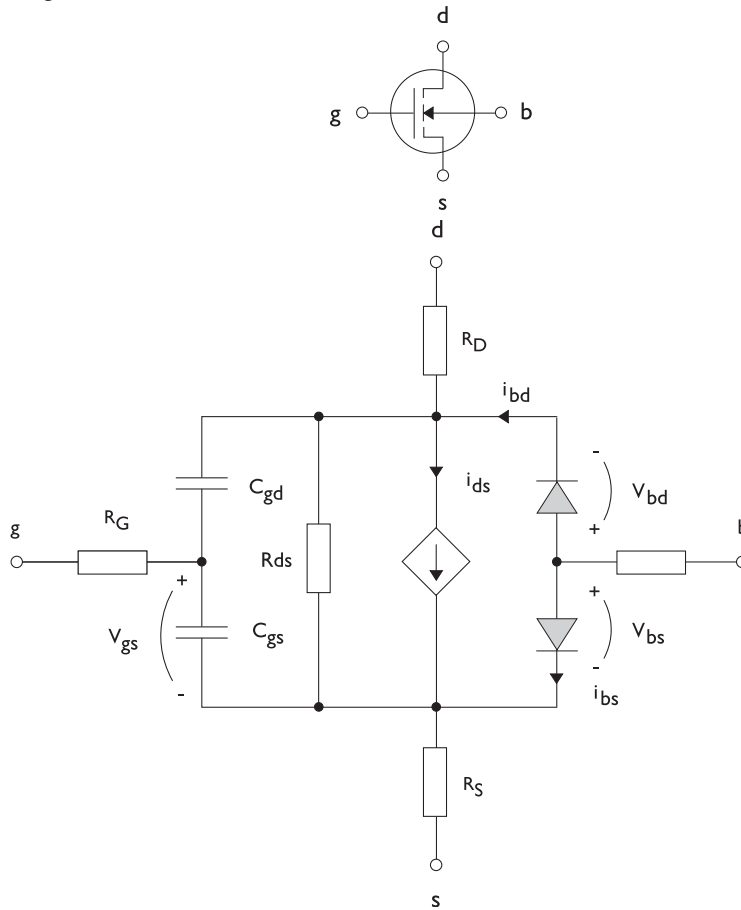


Figure 4-2: A circuit for the MOSFET transistor.

The following equations are used to compute the relations between currents and voltages in the circuit.

$$i_{ds} = \begin{cases} \frac{WK_P}{L} \frac{1}{2} (1 + \Lambda v_{ds}) v_{ds} (2v_{th} - v_{ds}) & v_{ds} < v_{th} \\ \frac{WK_P}{L} \frac{1}{2} (1 + \Lambda v_{ds}) v_{th}^2 & v_{ds} \geq v_{th} \\ 0 & v_{ds} < v_{th} \leq 0 \end{cases}$$

$$v_{th} = v_{gs} - (V_{TO} + \Gamma(\sqrt{\Phi} - v_{bs} - \sqrt{\Phi}))$$

$$i_{bd} = I_S \left(e^{\frac{v_{bd}}{NV_T}} - 1 \right)$$

$$i_{bs} = I_S \left(e^{\frac{v_{bs}}{NV_T}} - 1 \right)$$

$$V_T = \frac{k_B T_{NOM}}{q}$$

There are also several capacitances between the terminals

$$C_{gd} = C_{gd0} W$$

$$C_{gs} = C_{gs0} W$$

$$C_{jbd} = C_{BD} \times \begin{cases} \left(1 - \frac{v_{bd}}{P_B} \right)^{-M_J} & v_{bx} < F_C P_B \\ (1 - F_C)^{-1-M_J} \left(1 - F_C (1 + M_J) + M_J \frac{v_{bx}}{P_B} \right) & v_{bx} \geq F_C P_B \end{cases}$$

The model parameters are as follows:

TABLE 4-2: MOSFET TRANSISTOR MODEL PARAMETERS.

PARAMETER	DEFAULT	DESCRIPTION
C_{BD}	0 F/m	Bulk-drain zero-bias capacitance
C_{GDO}	0 F/m	Gate-drain overlap capacitance
C_{GSO}	0 F/m	Gate-source overlap capacitance
F_C	0.5	Capacitance factor
I_S	1e-13 A	Bulk junction saturation current
K_P	2e-5 A/V ²	Transconductance parameter
L	50e-6 m	Gate length
M_J	0.5	Bulk junction grading coefficient

TABLE 4-2: MOSFET TRANSISTOR MODEL PARAMETERS.

PARAMETER	DEFAULT	DESCRIPTION
N	1	Bulk junction ideality factor
P_B	0.75 V	Bulk junction potential
R_B	0 Ω	Bulk resistance
R_D	0 Ω	Drain resistance
R_{DS}	Inf (Ω)	Drain-source resistance
R_G	0 Ω	Gate resistance
R_S	0 Ω	Source resistance
T_{NOM}	298.15 K	Device temperature
V_{TO}	0 V	Zero-bias threshold voltage
W	50e-6 m	Gate width
Γ (GAMMA)	1 $\text{V}^{0.5}$	Bulk threshold parameter
Φ (PHI)	0.5 V	Surface potential
Λ (LAMBDA)	0 1/V	Channel-length modulation

Diode

Figure 4-3 illustrates equivalent circuit for the diode.

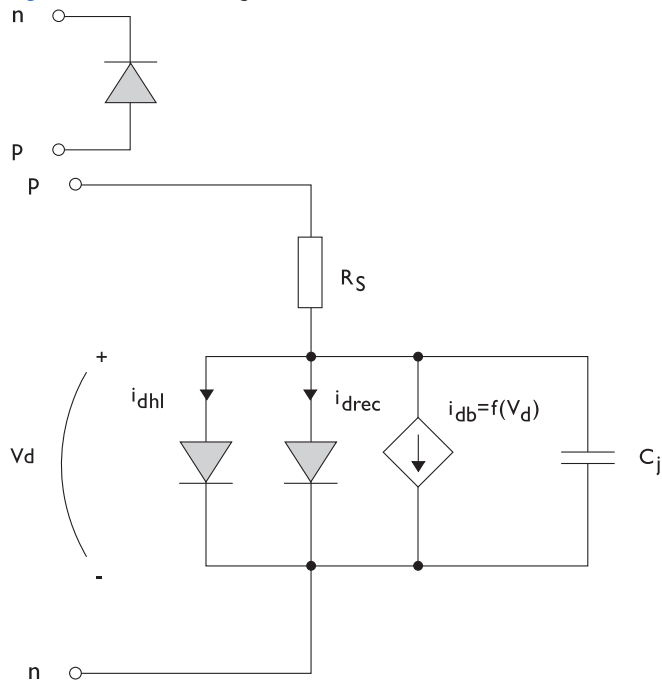


Figure 4-3: A circuit for the diode.

The following equations are used to compute the relations between currents and voltages in the circuit.

$$\begin{aligned}
i_d &= i_{dhl} + i_{drec} + i_{db} + i_c \\
i_{dhl} &= I_S \left(e^{\frac{v_d}{N V_T}} - 1 \right) \frac{1}{\sqrt{1 + \frac{I_S}{I_{KF}} \left(e^{\frac{v_d}{N V_T}} - 1 \right)}} \\
i_{drec} &= I_{SR} \left(e^{\frac{v_d}{N_R V_T}} - 1 \right) \\
i_{db} &= I_{BV} e^{\frac{v_d + B_V}{N_{BV} V_T}} \\
C_j &= C_{J0} \times \begin{cases} \left(1 - \frac{v_d}{V_J} \right)^{-M} & v_d < F_C V_J \\ (1 - F_C)^{-1-M} \left(1 - F_C (1 + M) + M \frac{v_d}{V_J} \right) & v_d \geq F_C V_J \end{cases} \\
V_T &= \frac{k_B T_{NOM}}{q}
\end{aligned}$$

where the following model parameters are required.


TABLE 4-3: DIODE TRANSISTOR MODEL PARAMETERS.

PARAMETER	DEFAULT	DESCRIPTION
B_V	Inf (V)	Reverse breakdown voltage
C_{J0}	0 F	Zero-bias junction capacitance
F_C	0.5	Forward-bias capacitance coefficient
I_{BV}	1e-09 A	Current at breakdown voltage
I_{KF}	Inf (A)	Corner for high-current roll-off
I_S	1e-13 A	Saturation current
M	0.5	Grading coefficient
N	1	Ideality factor
N_{BV}	1	Breakdown ideality factor
N_R	2	Recombination ideality factor
R_S	0 Ω	Series resistance
T_{NOM}	298.15 K	Device temperature
V_J	1.0 V	Junction potential

Reference for the Electrical Circuit Interface

1. P. Antognetti and G. Massobrio, *Semiconductor Device Modeling with Spice*, 2nd ed., McGraw Hill, 1993.

Chemistry and Reaction Engineering Interfaces

This chapter describes the **Chemistry (chem)** and **Reaction Engineering (re)** interfaces, available in the **Chemical Species Transport** branch ().


In this chapter:

- [Overview of the Reaction Engineering and Chemistry Interfaces](#)
- [Theory for the Reaction Engineering and Chemistry Interfaces](#)
- [The Reaction Engineering Interface](#)
- [The Chemistry Interface](#)

Overview of the Reaction Engineering and Chemistry Interfaces

The **Reaction Engineering** and **Chemistry** interfaces share many common features and functionality for defining species and reactions. The main difference is that the **Reaction Engineering** interface always is defined within the context of a (zero dimensional) *reactor model*, solving for a number of species dependent variables and an optional heat balance, whereas the **Chemistry** interfaces solely defines a number of *variable expressions*, based on species and reactions, that can be used when coupling the **Chemistry** interface to, for instance, a space-dependent mass transport model.

THE REACTION ENGINEERING INTERFACE

The [Reaction Engineering Interface](#) () includes all of the tools required to simulate chemical reaction kinetics in well-defined environments. This includes the automatic set up and simulation of reversible, equilibrium, and irreversible reactions in volumes or on surfaces. A library of predefined reactors is also available, including batch, continuous stirred-tank, semibatch, and plug flow reactors (see [Reactor Types in the Reaction Engineering Interface](#)). In addition, the Parameter Estimation feature makes it possible to evaluate kinetic and model parameters from experimental data.




Use the [Generate Space-Dependent Model](#) node to create a space-dependent model based on your model created in the Reaction Engineering interface. This automatically sets up the mass balances and source terms for systems where reactions occur, with a copy of all and your original species and reaction definitions recreated in separate a Chemistry node.

The Reaction Engineering interface can also be used for defining and simulating thermodynamic data.

Interfaces to internal or external thermodynamic packages (such as CAPE-OPEN compliant packages), and an import feature for CHEMKIN[®] files, mean that the thermodynamic properties within reaction kinetics, as well as mass and heat transfer applications, can be described by empirical relations and algebraic expressions. Also see the [Theory for the Reaction Engineering and Chemistry Interfaces](#).

THE CHEMISTRY INTERFACE

The [Chemistry Interface](#) () is a tool for generating a set of variables to be used for modeling chemical species and reactions systems. The variables are generated from species and reaction properties and can be divided in two categories:

- Rate expressions and heat sources for use in mass and heat balances
- Material property variables (mixture density, diffusivities, viscosity, and so on) for use in space-dependent transport equations.

The **Chemistry** interface is also created when the [Generate Space-Dependent Model](#) feature is used in [The Reaction Engineering Interface](#), collecting all mixture variables and properties for use in a space-dependent model.

Using the Reaction Node

In each [Reaction](#) node, specify the reaction **Formula** (chemical equation) and **Reaction type** of a single chemical equation.

For each reaction formula entered, specify the reaction type with a delimiter separating the two sides of the equation:

- \rightleftharpoons denotes a reversible reaction
- \Rightarrow denotes an irreversible reaction
- $=$ denotes a reaction at chemical equilibrium

It is also possible to adjust the reaction type with the **Reaction type** list (Figure 5-1).

Settings
Reaction

Label: 1: roh + H+ => ren + H2O + H+

Reaction Formula Balance

Formula:
roh + H+ => ren + H2O + H+ Apply

Reaction type:
Irreversible

$$R_i = \sum_j \nu_{ij} r_j$$

Reaction Rate

Mass action law

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}}$$

Overall forward reaction order: 2

Rate Constants

☐ Use Arrhenius expressions

Forward rate constant:
k^f [7.45e-3[m³/(s*mol)]] m³/(mol*s)

Figure 5-1: After adding a Reaction node, enter the chemical reaction formula (chemical equation) and specify the reaction type.

Right-click any **Reaction** node to disable and enable the corresponding node in the **Model Builder**. Creating reaction subsets in this way is a straightforward approach to investigate the influence of individual reactions on the overall reaction system. Species that take part only in deactivated reactions are automatically deactivated, as indicated by the unavailable **Species** feature nodes. If a reaction is deleted, the interface automatically deletes those species that take part only in the deleted reactions.

ABOUT REACTION IDENTIFICATION NUMBERS, VARIABLE SCOPE, AND LABELING

When reaction formulas are entered, each reaction is associated with a unique ID (identification) number (Figure 5-2). The ID number is not a row number but rather an absolute reference number to a given reaction. This means that a reaction keeps its ID number, even if reactions are deleted with a lower number. Furthermore, constants

and expressions within fields associated with a given reaction are also indexed with the reaction number.

The **Name** prepended to the variable name is called the variable scope. Defaults are **re** and **chem** for the Reaction Engineering and Chemistry interface, respectively. All variables set up by the interface are given the same scope. The variable scope can be useful to couple the equations of different physics interfaces.

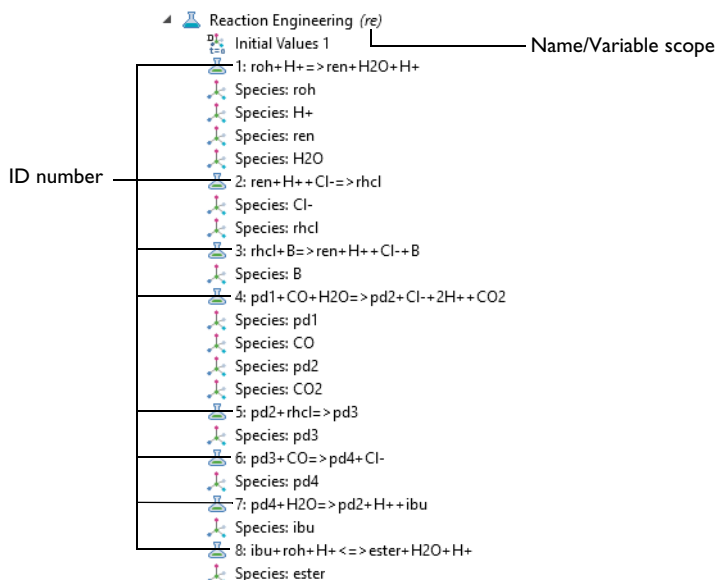


Figure 5-2: The ID number of each Reaction node is displayed in front of the reaction formula.

As a general labeling rule, the variable name that refers to the contents of a field associated with a **Reaction** node is given by the physics interface **Name**, followed by the field name, and ends with the reaction ID number. For example, the contents of the reaction rate field **r** for Reaction 1 is assigned the variable name **re.r_1**.



For an example of how to use variables with scope, see *Tank Series with Feedback Control*: Application Library path
**Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/
 tankinseries_control**

Using the Species Node

The [Reaction Engineering Interface](#) and [The Chemistry Interface](#) generate **Species** nodes in the **Model Builder** based on the chemical equations entered in the **Settings** window for **Reaction**.

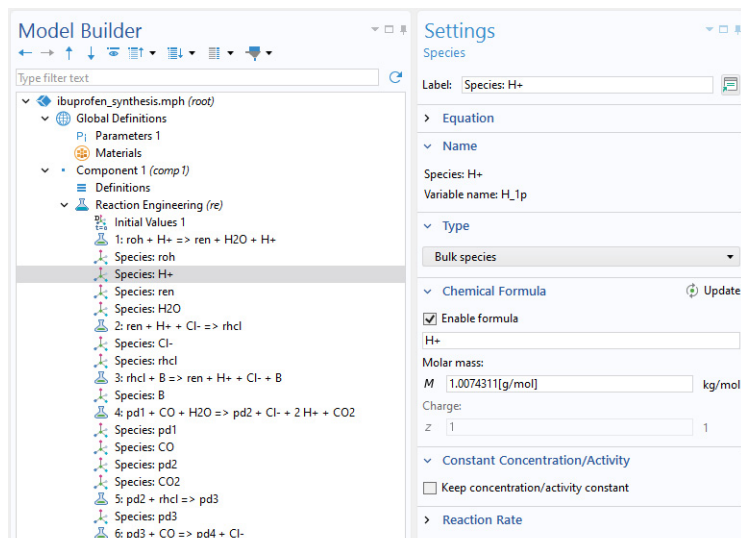


Figure 5-3: Species nodes are generated automatically as chemical equations are entered in the Reaction nodes.

As with [Reaction](#) features you can add, remove, or deactivate [Species](#) features by right-clicking a node in the Model Builder. Deactivation of a species automatically deactivates any reactions in which the species is participating.

In the **Reaction Rate** section it is possible to alter the definition of the reaction rate of the species. This will override the settings in the [Reaction](#) feature, where the rate is defined by the stoichiometry of the reaction(s) in which the species participates.

It is also possible to add individual **Species** nodes with either reactive or nonreactive species.

CHOOSING THE SPECIES TYPE

For each species entered, it is possible to change its characteristics by selecting its species type — **Bulk species**, **Surface species**, or **Solvent**.

The **Type** selection has implications in the calculation of thermodynamic and transport properties.

Bulk species and **Surface species**, defined per reactor volume and area, respectively, set the mixture's physical properties dependent upon its composition. However, configuring a species as a **Solvent** sets the physical properties of the reacting fluid mixture equal to those of the solvent species; specifically, its density, heat capacity, viscosity, and thermal conductivity. The interface also implements a solute-solvent approximation for the interaction of species in the fluid and describes the transport properties accordingly. In material balances this means that the diffusion coefficient is independent of any of the solute's concentrations, because every solute only interacts with solvent molecules, regardless of the concentration. In addition, the convective term in the flux of species is directly given by the velocity field of the solvent multiplied by the solute concentration.

The **Type** has implications on the [Generate Space-Dependent Model](#) procedure since it determines whether interfaces using a solvent-solute approximation of the reacting fluid mixture (as in [The Transport of Diluted Species Interface](#)) or a full multicomponent description of the reacting fluid mixture (as in [The Transport of Concentrated Species Interface](#)) should be generated.

Furthermore, the **Type** affects the reaction kinetics. **Solvent** sets the species' concentration to a constant value (the initial species concentration). The Reacting Engineering interface does not formulate a mass balance for the solvent species. This setting corresponds to situations where the solvent does not take part in chemical reactions at all, or where it reacts but is present in large excess.

VALID SPECIES NAMES

Valid species names consist of a case-sensitive combination of letters, numbers, charge indication and phase indication. With the exception of the “+” and “-” signs, the caret character “^”, underscore “_”, and the enclosing characters “()[]{}”, special characters are not allowed. In addition, the first character in a species name must be a letter, or enclosing character, to avoid confusion with the stoichiometric coefficients in the reaction formula.

Charge is indicated in one of the following ways:

- Fe++, Fe(++), Fe(2+)
- Fe^++, Fe^(++), Fe^(2+), Fe^2+


The charge indication, for example (++), is placed last in the species name, but before any phase indication. The charge is automatically read from the species **Name** field, or **Chemical Formula** field, and entered in the **Charge** field in the associated Species feature.

A valid phase indication consists of a valid species name followed by a valid phase. The phase should be placed last. For example, water in gaseous form is written “H₂O(g)”, and a divalent cation of iron in water can be written “Fe²⁺(aq)”. Valid phases are:

- (g), for gas or vapor
- (l), for liquid
- (s), for solid
- (aq), for aqueous solution
- (ads), for adsorbed/surface species
- (cd), for condensed phase (solid or liquid)
- (fl), for fluid (gas or liquid)
- (lc), for crystalline liquid
- (cr), for crystalline solid
- (am), amorphous solid
- (vit), vitreous substance (glass)
- (mon), for monomeric form
- (pol), for polymeric form
- (sln), for solution

Using the phases **(ads)**, **(s)**, **(l)**, **(aq)**, or **(g)** creates adsorbed, solid, liquid, aqueous, or gaseous species with variable names; `speciesname_surf`, `speciesname_solid`, `speciesname_liquid`, `speciesname_aq`, or `speciesname_gas`, respectively. The **Type** field in the Species feature, is filled in automatically depending on which phase that was used. The phases **(s)**, **(l)**, and **(g)** give rise to **Bulk species**, while a species with phase indication **(ads)** results in a **Surface species**. **(aq)** gives rise to aqueous species. Note that the [Equilibrium Species Vector](#) remains the same despite the presence of any gaseous or liquid species in the system.


Similar to the labeling rule applying to Reaction nodes, the variable name referring to the contents of a field associated with a Species node is given by the interface **Name**, followed by the field name, and ending with the species name. For example, the contents of the **Rate expression** field **R** for the species roh is assigned the variable name `re.R_roh` (for the Reaction Engineering interface). Access the definition of all the variables used by a specific node by displaying the **Equation View** node. To display the

node, click the **Show More Options** button () and select **Equation View** in the **Show More Options** dialog.



- [Theory for the Reaction Engineering and Chemistry Interfaces](#)
- [Variable Naming Convention and Namespace](#)

Using the Equation View Node — Reactions and Species

To display the **Equation View** node, click the **Show More Options** button () and select **Equation View** in the **Show More Options** dialog. Expand any node, for example the [Reaction](#) or [Species](#) nodes, and click the **Equation View** to see the page where the definition of all the variables used by a specific node are listed ([Figure 5-4](#)).

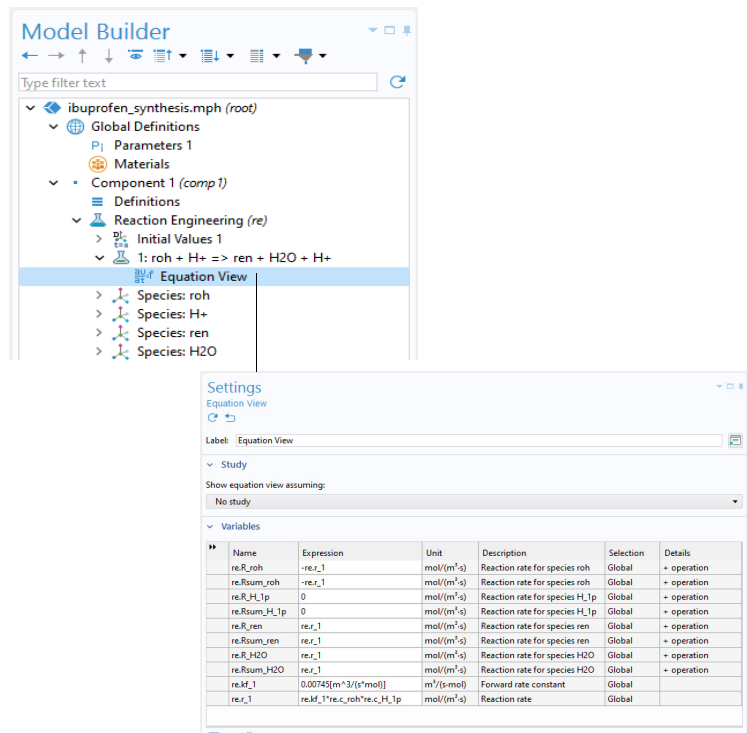


Figure 5-4: The definition of variables used by a node are accessible through the Equation View.

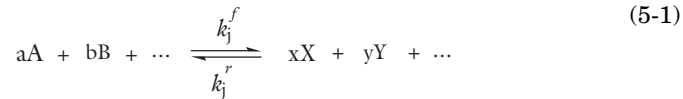
Theory for the Reaction Engineering and Chemistry Interfaces

The [Reaction Engineering Interface](#) and [The Chemistry Interface](#) theory is described in this section.

- [Reactor Types in the Reaction Engineering Interface](#)
- [Transport Properties](#)
- [CHEMKIN Data and NASA Polynomials](#)
- [Working with Predefined Expressions](#)
- [References for the Reaction Engineering Interface](#)

Reaction Kinetics and Rate Expressions

The modeling of reactions in COMSOL uses the mass action law by default. Consider a general reaction belonging to a set of j reactions and involving i species:



For such a reaction set, the reaction rates r_j (SI unit: $\text{mol}/(\text{m}^3 \cdot \text{s})$) can be described by the mass action law:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}} \quad (5-2)$$

Here, k_j^f and k_j^r denote the forward and reverse rate constants, respectively. The concentration of species i is denoted as c_i (SI unit: mol/m^3). The stoichiometric coefficients are denoted ν_{ij} , and are defined as being negative for reactants and positive for products. In practice, a reaction seldom involves more than two species colliding in a reacting step, which means that a kinetic expression is usually of order 2 or less (with respect to the involved concentrations).

In addition to the concentration dependence, the temperature dependence of reaction rates can be included by using the predefined Arrhenius expression for the rate constants:

$$k = A \left(\frac{T}{T_{\text{ref}}} \right)^n \exp \left(-\frac{E}{R_g T} \right) \quad (5-3)$$

Here, A denotes the frequency factor, n the temperature exponent, E the activation energy (SI unit: J/mol) and R_g the gas constant, 8.314 J/(mol·K). The pre-exponential factor, including the frequency factor A and the temperature factor T^n , is given the units (m³/mol) ^{$\alpha-1$} /s, where α is the order of the reaction (with respect to volumetric concentrations).

The default settings for the reaction given by [Equation 5-1](#) and assuming equilibrium, yields the equilibrium expression in [Equation 5-4](#):

$$K_c = \frac{c_X^x c_Y^y \dots}{c_A^a c_B^b \dots} \quad (5-4)$$

In the case of reversible reactions, it is also possible to make use of equilibrium relationships in order to indirectly calculate reaction constants. For example, calculate the reverse rate constant from the equilibrium condition in this way:

$$k^r = \frac{k^f}{K_c} \quad (5-5)$$

The Equilibrium Constant

In general, chemical equilibrium is reached when the Gibbs free energy of the system is minimized. The Gibbs free energy of is defined as

$$G(T, P) = U + PV - TS = H - TS \quad (5-6)$$

where U is the internal energy, P is pressure, V is volume, T is temperature, S is entropy and H is enthalpy of the system. For a closed system

$$dU = \delta Q + \delta W = TdS - PdV \quad (5-7)$$

where δQ is (reversible) heat transfer to the fluid and δW is (pressure) work in the system. The change in Gibbs free energy can be written as

$$dG = TdS - PdV + PdV + VdP - TdS - SdT = VdP - SdT \quad (5-8)$$

Chemical potential μ_i is defined as partial molar Gibbs energy for species

$$\mu_i = \left(\frac{\partial G}{\partial n_i} \right)_{T, P, n_i \neq n_j} \quad (5-9)$$

where n is the number of mole of species i in the system. At constant temperature, this expression can be integrated as a function of pressure

$$\int_{\mu_i^o}^{\mu_i} d\mu = \int_{P^o}^{P_i} \bar{v}_i dP \quad (5-10)$$

where v is molar volume and μ_i^o is chemical potential of species at standard state. For an ideal gas this can be expressed as

$$\mu_i - \mu_i^o = R_g T \ln \left(\frac{P_i}{P^o} \right) \quad (5-11)$$

The equilibrium criterion can be written as

$$\sum_i \nu_i \mu_i = 0 \quad (5-12)$$

where ν_i is the stoichiometric coefficient and μ_i is the chemical potential of species i in the reaction. We can evaluate the chemical potential as partial molar Gibbs energy of species in mixture as

$$\mu_i - \mu_i^o = R_g T \ln \left(\frac{\hat{f}_i}{f_i^o} \right) \quad (5-13)$$

where \hat{f}_i is the fugacity of species i in the mixture, and f_i^o is the fugacity of pure species in the standard state. Equation 5-12 can be rewritten as

$$\sum_i \nu_i \mu_i^o + R_g T \ln \prod_i \left(\frac{\hat{f}_i}{f_i^o} \right)^{\nu_i} = 0 \quad (5-14)$$

The equilibrium constant for the reaction, K , is defined as

$$K(T) = \exp \left(\frac{-\Delta G_{\text{rxn}}^o}{RT} \right) = \prod_i a_i^{\nu_i} = \prod_i \left(\frac{\hat{f}_i}{f_i^o} \right)^{\nu_i} \quad (5-15)$$

where a_i is the activity of species in the system.

ΔG_{rxn}^o is the Gibbs free energy of reaction (including formation terms) which is defined, in accordance with Equation 5-6, as

$$\Delta G_{rxn}^o = \Delta H_{rxn}^o - T\Delta S_{rxn}^o \quad (5-16)$$

the enthalpy of reaction, ΔH_{rxn}^o , and entropy of reaction, ΔS_{rxn}^o , both at a given temperature T is defined as

$$\Delta H_{rxn}^o(T) = \sum_i \nu_i \left(\Delta H_{f,i}^o + \int_{T^o}^T C_{p,i} dT \right) \quad (5-17)$$

$$\Delta S_{rxn}^o(T) = \sum_i \nu_i \left(S_{abs,i} + \int_{T^o}^T \frac{C_{p,i}}{T} dT \right) \quad (5-18)$$

Here T^o is the temperature at standard state. $\Delta H_{f,i}^o$ and $S_{abs,i}$ are the standard enthalpy of formation and absolute entropy for each species (these data are available in the COMSOL database).

ACTIVITY

Activity of species, a_i is defined by Equation 5-13 as

$$a_i = \exp \left(\frac{\mu_i - \mu_i^o}{R T} \right) \quad (5-19)$$

Activity depends on the choice of an arbitrary standard state. The standard state of pure species is usually at 10^5 Pa and for solute in solution is based on hypothetical molality or amount concentration also referred as infinite dilute behavior.

The activity of a species in a mixture is expressed by relationship between dimensionless activity coefficients, γ_i , and measured amount of the species in the system.

$$a_i = \gamma_{x,i} x_i = \gamma_{c,i} \frac{c_i}{c_{ref}} \quad (5-20)$$

Activity coefficients are usually estimated by [Activity Coefficient Models](#).

Gas Phase

The standard state is the pure species at ideal gas condition, 1 atm and the equilibrium temperature. Activity of species in mixture is expressed by:

$$a_i = \frac{\hat{f}_i}{f_i^o} = \frac{y_i \hat{\phi}_i P}{P^o} \quad (5-21)$$

where \hat{f}_i and $\hat{\phi}_i$ are the fugacity and fugacity coefficient of species i in the mixture.

Liquid Phase

The standard state is pure liquid species at 1 atm and equilibrium temperature. The fugacity of a species in a mixture is given by

$$\hat{f}_i = y_i \gamma_i f_i \quad (5-22)$$

where γ_i is the activity coefficient of species in the mixture and f_i is the fugacity of pure species at the equilibrium temperature and pressure. The activity is expressed by

$$a_i = \frac{y_i \gamma_i f_i}{f_i^o} \quad (5-23)$$

where f_i^o is the fugacity of pure species at the equilibrium temperature and 1 atm. The ratio f_i/f_i^o is given by

$$\frac{f_i}{f_i^o} = \exp\left(\frac{v_i}{R_g T}(P - P_i^{\text{sat}})\right) \quad (5-24)$$

where v_i is the partial molar volume of species and P^{sat} is species saturated vapor pressure. For liquids it is a weak function of pressure, and can be assumed to be 1 unless at high pressure.

Dilute Solutions

The concentration can in the case of nonideal mixtures be replaced with the activity. In these interfaces, the dimensionless activity (a_i) depend on species concentration (c_i), activity coefficient (γ_i), and the standard state concentration ($c_{0s} = 1 \text{ mol/m}^3$).

$$a_i = \frac{c_i}{c_{0s}} \gamma_i \quad (5-25)$$

Additionally, an effective species concentration ($c_{e,i}$) (SI unit: mol/m^3) is used in the reaction rates ([Equation 5-2](#)) when activities are utilized.

$$c_{e,i} = c_i \gamma_i = a_i c_{0s} \quad (5-26)$$

AUTOMATICALLY DEFINED EQUILIBRIUM CONSTANTS

Below, the automatically defined equilibrium constants are defined in terms of the equilibrium expression K_c

$$K_c = \prod_i c_i^{v_i} = \frac{\prod_{i \in \text{prod}} c_i^{v_i}}{\prod_{i \in \text{react}} c_i^{-v_i}} \quad (5-27)$$

Gas Phase

Inserting Equation 5-21 in Equation 5-15 gives:

$$K(T) = K_{\text{eq}} \prod_i \left(\frac{\hat{\phi}_i P}{c_{\text{sum}} P^0} \right)^{v_i} \quad (5-28)$$

where for ideal mixtures, the fugacity coefficients ϕ_i are equal to 1.

Liquid Phase

For low and moderate pressure, the equilibrium constant can be reformulated by substitution of Equation 5-23 to Equation 5-15 as:

$$K(T) = K_c \prod_i \left(\frac{\gamma_i}{c_{\text{sum}}} \right)^{v_i} \quad (5-29)$$

Handling of Equilibrium Reactions

EXAMPLE I

The following short example illustrates how the Reaction Engineering interface and the Chemistry interface handle equilibrium reactions in the formulation of the material balance equations.

Consider the reaction:



According to Equation 5-2 the reaction rate (SI unit: mol/(m³·s)) is formulated as:

$$r = k^f c_A - k^r c_B$$

where c_A and c_B (SI unit: mol/m³) are the concentrations of A and B , and k^f and k^r (SI unit: 1/s) are the forward and reverse rate constants, respectively. The net rate expressions with respect to species A and B are then:

$$R_A = -k^f c_A + k^r c_B = -r$$

$$R_B = k^f c_A - k^r c_B = r$$

Assuming the reaction in [Equation 5-30](#) is at equilibrium, the reaction rate r is 0:

$$r = k^f c_A - k^r c_B = 0$$

The relationship between the forward and reverse reaction rates in [Equation 5-30](#) is given by the following ratio:

$$K^{\text{eq}} = \frac{k^f}{k^r} = \frac{c_B}{c_A} \quad (5-31)$$

The Reaction Engineering interface also sets up mass balances that are solved. The general material balances for species A and B , respectively, are:

$$\frac{\partial c_A}{\partial t} = R_A = -r \quad (5-32)$$

$$\frac{\partial c_B}{\partial t} = R_B = r \quad (5-33)$$

The rate of consumption of species A equals the production rate of species B , as shown in [Equation 5-32](#) and [Equation 5-33](#).

With the combined information in [Equation 5-32](#), [Equation 5-33](#), and [Equation 5-31](#), the Reaction Engineering interface is able to define the mass balances for the equilibrium system without the reaction rate expressions. The equation system solved for becomes:

$$\frac{\partial}{\partial t}(c_A + c_B) = 0 \quad (5-34)$$

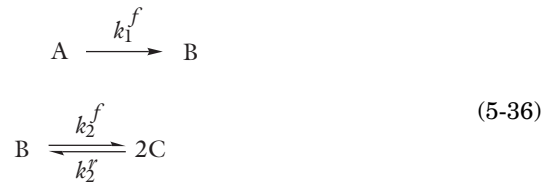
$$K^{\text{eq}} = \frac{c_B}{c_A} \quad (5-35)$$

In general, for a system of reactions contributing to k mass balances and with j reactions being at equilibrium, the reduced system of equations to be solved is composed of $k - j$ mass balances and j equilibrium expressions. The elimination process producing the above system of equations is automated, allowing simple modeling of chemical equilibrium reactions together with irreversible and/or reversible reactions.

EXAMPLE II

This example shows how equilibrium reactions are considered in the Reaction Engineering interface using the [Equilibrium Species Vector](#) section.

If two nonequilibrium reactions are taking place in a perfectly mixed isothermal reactor of constant volume:



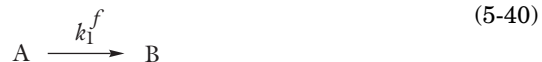
the corresponding mass balances are:

$$\frac{d}{dt}c_A = -r_1 \quad (5-37)$$

$$\frac{d}{dt}c_B = r_1 - r_2 \quad (5-38)$$

$$\frac{d}{dt}c_C = 2r_2 \quad (5-39)$$

Now compare [Equation 5-37](#), [Equation 5-38](#), and [Equation 5-39](#) with the balance equations that the physics interface sets up for the related chemistry, where the second reaction is instead an equilibrium reaction:



In contrast to the reversible reaction given by [Equation 5-36](#), to make use of the information contained in the equilibrium relation, the mass balances must be reformulated. Mass balances set up for the reactions given by [Equation 5-40](#) and [Equation 5-41](#) are then:

$$\frac{d}{dt}c_A = -r_1$$

$$\frac{d}{dt}(2c_B + c_C) = 2r_1 \quad (5-42)$$

$$K_2^{\text{eq}} = \frac{c_C^2}{c_B} \quad (5-43)$$

The equilibrium expression ([Equation 5-43](#)) introduces an algebraic relationship between the species' concentrations.

Two species, B or C, can be set as Predefined Dependent Species in the [Equilibrium Species Vector](#) section. Selecting B as the dependent species solves [Equation 5-42](#) for the concentration of C, while B is computed from [Equation 5-43](#).

Reactor Types in the Reaction Engineering Interface

MASS BALANCE

The mass balances that are set up in the Reaction Engineering interface are simplified versions of the general mass transport equation. The main assumption is that the reactor is perfectly mixed, meaning that any variations in compositions within the reactor are neglected.



- [Mass Balance Equation](#)
-

ENERGY BALANCE

The energy balances solved in the Reaction Engineering interface are derived from the general energy balance of a system. The utilized equation follows the perfect mixing assumption and is dependent on the selected reactor as described below.



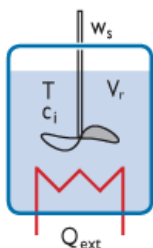
Theory for Heat Transfer

The following reactor types are available in the Reaction Engineering interface (the Chemistry interfaces does not contain reactor models):

- Batch
- Batch, Constant Volume
- CSTR, Constant Mass/Generic
- CSTR, Constant Volume
- Semibatch
- Plug Flow

BATCH

In the batch reactor no mass enters or leaves the system. Common for all reactor models is that reacting fluids in the gas phase are assumed to behave as ideal gases. Liquid mixtures are assumed to be ideal and incompressible.



The species mass balances are given by:

$$\frac{d(c_i V_r)}{dt} = V_r R_i \quad (5-44)$$

which takes into account the effect of changing volume. In Equation 5-44, c_i (SI unit: mol/m^3) is the species molar concentration, V_r (SI unit: m^3) denotes the reactor volume, and R_i (SI unit: $\text{mol}/(\text{m}^3 \cdot \text{s})$) is the species rate expression.

For an ideal reacting gas, the energy balance is:

$$V_r \sum_i c_i C_{p,i} \frac{dT}{dt} = Q + Q_{\text{ext}} + V_r \frac{dp}{dt} \quad (5-45)$$

In Equation 5-45, $C_{p,i}$ (SI unit: J/(mol·K)) is the species molar heat capacity, T (SI unit: K) is the temperature, and p (SI unit: Pa) the pressure. On the right-hand side, Q (SI unit: J/s) is the heat due to chemical reaction, and Q_{ext} (SI unit: J/s) denotes heat added to the system. The heat of reaction is:

$$Q = -V_r \sum_j H_j r_j$$

where H_j (SI unit: J/mol) is the enthalpy of reaction, and r_j (SI unit: mol/(m³·s)) the reaction rate.

For an incompressible and ideally mixed reacting liquid, the energy balance is:

$$V_r \sum_i c_i C_{p,i} \frac{dT}{dt} = Q + Q_{\text{ext}} \quad (5-46)$$



Ibuprofen Synthesis: Application Library path
**Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/
 ibuprofen_synthesis**

BATCH, CONSTANT VOLUME

The constant volume batch reactor is the default reactor. It assumes a closed, perfectly mixed system of constant volume. The species mass balances are:

$$\frac{dc_i}{dt} = R_i$$

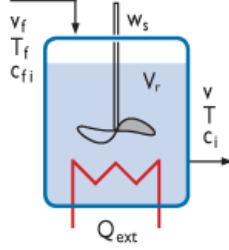
For an ideal reacting gas, the energy balance is given by Equation 5-45. For an incompressible and ideally mixed reacting liquid, the energy balance is given by Equation 5-46.



Neutralization of Chlorine in a Scrubber: Application Library path
**Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/
 chlorine_scrubber**

CSTR, CONSTANT MASS/GENERIC

The continuous stirred tank reactor (CSTR) has reacting species entering and leaving the reactor by means of inlet and outlet streams. The reactor is again assumed to be perfectly mixed, so that the species concentrations of the exit stream are the same as the concentrations in the reactor volume.



The species mass balances for the CSTR are given by:

$$\frac{d(c_i V_r)}{dt} = \sum_m v_{f,m} c_{f,m} - v c_i + R_i V_r \quad (5-47)$$

In Equation 5-47, $c_{f,m}$ (SI unit: mol/m³) is the species molar concentration of the associated feed inlet stream $v_{f,m}$ (SI unit: m³/s). V_r (SI unit: m³) denotes the reactor volume and is a function of time.

The reactor volume as a function of time is given by:

$$\frac{dV_r}{dt} = \sum_m v_{f,m} - v + v_p \quad (5-48)$$

In Equation 5-48, v_p (SI unit: m³/s) denotes the volumetric production rate. It is given by Equation 5-49 for ideally mixed liquids and by Equation 5-50 for ideal gases.

$$v_p = V_r \sum_i \frac{R_i M_i}{\rho_i}, \quad R_i = \sum_j v_{ij} r_j \quad (5-49)$$

$$v_p = \frac{R_g T}{p} V_r \sum_i R_i \quad (5-50)$$

where v_{ij} is the stoichiometric coefficient of species i in reaction j , M_i (SI unit: kg/mol) denotes the species molecular weight, ρ_i (SI unit: kg/m³) the species density, and R_i (SI unit: mol/(m³·s)) is the reaction rate of species i .

When this reactor model is solved for constant mass, the reactor model assumes that the volumetric flow rate of the outlet stream, v (SI unit: m^3/s), is adjusted in such a way that the total mass of the reactor is held constant:

$$v = \frac{\sum v_{f,m} \rho_{f,m}}{\rho} \quad (5-51)$$

In contrast, when the model is set to be solved for generic conditions a specific outlet flow stream can be set.

The energy balance for an ideal reacting gas is:

$$V_r \sum_i c_i C_{p,i} \frac{dT}{dt} = Q + Q_{\text{ext}} + V_r \frac{dp}{dt} + \sum_m \sum_i v_{f,mi} c_{f,mi} (h_{f,mi} - h_i) \quad (5-52)$$

For an incompressible and ideally mixed reacting liquid, the energy balance is:

$$V_r \sum_i c_i C_{p,i} \frac{dT}{dt} = Q + Q_{\text{ext}} + \sum_m \sum_i v_{f,mi} c_{f,mi} (h_{f,mi} - h_i) \quad (5-53)$$



Ideal Stirred Tank Reactor System: Application Library path
**Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/
 tank_flow_system**

CSTR, CONSTANT VOLUME

This reactor type is a CSTR reactor where the reactor volume is constant.

The species mass balances are given by:

$$\frac{d(c_i V_r)}{dt} = \sum_m v_{f,m} c_{f,m} - v c_i + R_i V_r \quad (5-54)$$

Assuming constant reactor volume:

$$\frac{dV_r}{dt} = 0$$

and setting the volumetric outlet rate to:

$$v = \sum_m v_{f,m} + v_p \quad (5-55)$$

Equation 5-54 can be rewritten as:

$$V_r \frac{dc_i}{dt} = v_{f,i} c_{f,i} - \left(\sum v_{f,i} + v_p \right) c_i + R_i V_r \quad (5-56)$$

The volumetric production rate, v_p , is defined as in Equation 5-49 and Equation 5-50.

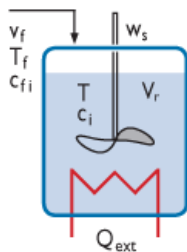
The energy balance is the same as for the CSTR with Constant Mass/Generic reactor type (Equation 5-53).



Startup of a Continuous Stirred Tank Reactor: Application Library
path **Chemical_Reaction_Engineering_Module/Tutorials/cstr_startup**

SEMI-BATCH

In the semibatch reactor, reactants enter the reactor by means of one or several feed inlet streams.



The species mass balances are given by:

$$\frac{d(c_i V_r)}{dt} = v_{f,i} c_{f,i} + R_i V_r \quad (5-57)$$

The reactor volume is a function of time given by:

$$\frac{dV_r}{dt} = \sum_m v_{f,m} + v_p \quad (5-58)$$

The volumetric production rate, v_p , is defined as in [Equation 5-49](#) and [Equation 5-50](#).

An energy balance over the Semibatch reactor results in the same energy balance expression as for the CSTR reactor types ([Equation 5-53](#)).

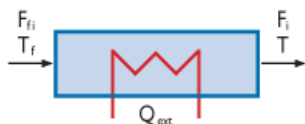


Semibatch Polymerization: Application Library path

**Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/
semibatch_polymerization**

PLUG FLOW

In the plug flow reactor the species concentrations and the temperature vary with position. For a tubular reactor configuration, plug flow assumes concentration and temperature gradients to only develop in the axial direction but not in the radial direction of the reactor.



The species mass balances are given by:

$$\frac{dF_i}{dV} = R_i \quad (5-59)$$

where F_i (SI unit: mol/s) is the species molar flow, V (SI unit: m^3) is the reactor volume, and R_i (SI unit: $\text{mol}/(\text{m}^3 \cdot \text{s})$) denotes the species rate expression.

In order to evaluate the rate expressions R_i , which are functions of the species concentrations, the physics interface calculates:

$$c_i = \frac{F_i}{v}$$

where v (SI unit: m^3/s) is the volumetric flow rate.

For liquids, the volumetric flow rate is given by:

$$v = \sum_i \frac{F_i M_i}{\rho_i}$$

where M_i (SI unit: kg/mol) denotes the species molecular weight and ρ_i (SI unit: kg/m³) the species density

For ideal gases:

$$v = \frac{R_g T}{p} \sum_i F_i$$

so that

$$c_i = \frac{p}{R_g T} \frac{F_i}{\sum_i F_i}$$

where p (SI unit: Pa) is the constant pressure.

Neglecting pressure drop, the energy balance for an ideal reacting gas, as well as an incompressible and ideally mixed reacting liquid is given by:

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q + Q_{\text{ext}} \quad (5-60)$$

Equation 5-60 is similar to the energy balance for the batch reactors (Equation 5-46), but with a reactor volume dependence instead of a time dependence.



Nonisothermal Plug-Flow Reactor: Application Library path
Chemical_Reaction_Engineering_Module/Tutorials/nonisothermal_plug_flow

Transport Properties

The Reaction Engineering Interface and The Chemistry Interface can calculate several transport properties that can be accessed in interfaces in space dependent models.

DIFFUSIVITY

The diffusivity is calculated in terms of binary diffusion coefficients. These are available for the following fluid mixtures:

Gases with or Without Solvent

The diffusion coefficients are calculated from the following expression based on kinetic gas theory (Ref. 7):

$$D_{AB} = 2.662821 \cdot 10^{-22} \cdot \frac{\sqrt{T^3(M_A + M_B)/(2 \cdot 10^3 M_A M_B)}}{p \sigma_A \sigma_B} \cdot \Omega_D^{-1} \quad (5-61)$$

Here, D_{AB} (SI unit: m^2/s) is the binary diffusion coefficient, M (SI unit: kg/mol) equals the molecular weight, T (SI unit: K) represents the temperature, p (SI unit: Pa) is the pressure, and σ (SI unit: m) equals the characteristic length of the Lennard–Jones/ Stockmayer potential. In addition, Ω_D is the collision integral, given by the relation of Neufeld and others (Ref. 6):

$$\Omega_D = \frac{c_1}{(T^*)^{c_2}} + \frac{c_3}{\exp(c_4 T^*)} + \frac{c_5}{\exp(c_6 T^*)} + \frac{c_7}{\exp(c_8 T^*)} \quad (5-62)$$

where the reduced temperature is:

$$T^* = T \frac{k_b}{\sqrt{\epsilon_A \epsilon_B}} \quad (5-63)$$

In Equation 5-62, c_x are empirical constants, μ_D is the species dipole moment value (SI unit: Cm) and ϵ/k_b (SI unit: K) the potential energy minimum value divided by Boltzmann's constant. Tabulated data in the literature frequently lists values of ϵ/k_b rather than ϵ . It should be noted that predefined expressions for binary diffusivities only treat ideal gas mixtures. Thus, these are applicable as input only for gases at moderate pressure in multicomponent diffusive transport models.

The binary diffusivity according to Equation 5-61 is also suited for gaseous species in solvent, simply by setting either the component A or B to the solvent. The binary diffusion coefficient is in this case equal to the diffusion coefficient of the bulk species.

Liquid with Solvent

The diffusivity of a species A in a solvent B is calculated with the Wilke–Chang equation (Ref. 8):

$$D_{AB} = 3.7 \cdot 10^{-15} \frac{(\phi_B M_B)^{1/2} T}{\mu_B V_{b,A}^{0.6}} \quad (5-64)$$

where μ_B (SI unit: Ns/m^2) denotes the solvent's dynamic viscosity (see Equation 5-69), and $V_{b,A}$ (SI unit: m^3/mol) equals the molar volume at the normal boiling point of the solute species. ϕ_B is the dimensionless association factor of the solvent, which by default is set to 1.

DYNAMIC VISCOSITY

The dynamic viscosities are computed for the following fluid mixtures:

Gases with Solvent

The dynamic viscosity of the mixture is assumed to be the same as that of the solvent. This is given by the kinetic gas theory (Ref. 6 and Ref. 7), with species i being the solvent:

$$\mu = 2.669 \cdot 10^{-6} \frac{\sqrt{T(M_i \cdot 10^3)}}{\sigma_i^2} \Omega_D^{-1} \quad (5-65)$$

In Equation 5-65, μ (SI unit: Ns/m^2) represents the dynamic viscosity, and Ω_D is the dimensionless collision integral given by:

$$\begin{aligned} \Omega_D = & b_1(T/(\epsilon_i/k_b))^{-b_2} + b_3[\exp(-b_4 T/(\epsilon_i/k_b))] \\ & + b_5[\exp(-b_6 T/(\epsilon_i/k_b))] + \frac{(4.998 \cdot 10^{-40})\mu_{D,i}^4}{k_b^2 T(\epsilon_i/k_b)\sigma_i^6} \end{aligned} \quad (5-66)$$

In Equation 5-65 and Equation 5-66, b_x are empirical constants, μ_D (SI unit: Cm) the species dipole moment value, and ϵ/k_b (SI unit: K) the potential energy minimum value divided by Boltzmann's constant. Tabulated data in the literature frequently lists values of ϵ/k_b rather than ϵ , and σ (SI unit: \AA) is the characteristic length value.

Gases without Solvent

The dynamic viscosity of gas mixtures without solvent are calculated according to Ref. 9 with the following expression:

$$\mu = \sum_{i=1}^n \left(\frac{\mu_i}{1 + \frac{1}{x_i} \sum_{j=1, j \neq i}^n x_j \phi_{ij}} \right) \quad (5-67)$$

where ϕ_{ij} is defined as:

$$\phi_{ij} = \frac{[1 + (\mu_i/\mu_j)^{0.5}(M_j/M_i)^{0.25}]^2}{(2\sqrt{2})[1 + M_i/M_j]^{0.5}} \quad (5-68)$$

In Equation 5-67 and Equation 5-68, x_i is the molar composition and μ_i is computed with Equation 5-65 for each of the species in the mixture.

Liquid with Solvent

The dynamic viscosity of the mixture is assumed to be the same as that of the solvent. An approximate expression for the temperature dependence of the dynamic viscosity is given by (Ref. 3):

$$\mu = 10^{-3} \left((\mu_{\text{ref}} 10^3)^{-0.2661} + \frac{T - T_{\text{ref}}}{223} \right)^{-3.758} \quad (5-69)$$

where μ (SI unit: Ns/m²) is the dynamic viscosity. As inputs for Equation 5-69, the physics interface takes the reference viscosity, μ_{ref} (SI unit: Pa·s) at the reference temperature T_{ref} (SI unit: K).

THERMAL CONDUCTIVITY

The thermal conductivity is calculated as well for some types of fluid mixtures:

Gas With or Without Solvent

The predefined expression for thermal conductivity comes from the Stiel–Thodos equation (Ref. 10), which is defined as:

$$k = \frac{\mu}{M} (1.15 C_p + 0.88 R_g) \quad (5-70)$$

where k (SI unit: W/(m·K)) is the thermal conductivity and C_p (SI unit: J/(mol·K)) denotes the molar heat capacity. Equation 5-70 is a function of viscosity, μ , as given by Equation 5-65. Equation 5-70 is directly used in the case of a solvent; all parameters being those of the solvent. Without a solvent, however, the following equation is also used:

$$k = \frac{1}{2} \left[\sum_{i=1} x_i k_i + \left(\sum_{i=1} \frac{x_i}{k_i} \right)^{-1} \right]$$

where k_i is the thermal conductivity of each species i and x_i the molar composition for each of the species in the mixture.

CHEMKIN[®] files can be used to import data for simulation of complex chemical reactions in the gas phase. These input files may contain three basic sets of information — chemical kinetics, species thermodynamic properties, and species transport properties for either volumetric or surface species. Use imported data to set up and do the following:

- Solve mass and energy balances for ideal reactor systems (reactors, semi-reactors, CSTRs, and plug flow reactors).
- Evaluate species transport properties as a function of reactor conditions.
- Evaluate mass, energy, and momentum balances for space-dependent models, and transfer them to COMSOL Multiphysics.

It is possible to read the input files for kinetics, thermodynamic, and transport properties independently and use these as separate data resources. For example, if a set of reactions is entered into the Reaction Engineering interface, species thermodynamic and transport data can be supplied by reading the appropriate input files. The full functionality of the physics interface is retained even after the import procedure. This means that all expressions and all data imported into the software are available for reference and for editing.

The following CHEMKIN files are compatible:

- Transport CHEMKIN files that supply data used to compute [Transport Properties](#).
- Thermodynamic CHEMKIN files containing data for Gordon and McBride or NASA polynomials ([Ref. 4](#)). These polynomials are denoted *NASA format* and compute the species' heat capacity, molar enthalpy, and molar entropy, in the manner of:

$$C_{p,i} = R_g(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4) \quad (5-71)$$

$$h_i = R_g\left(a_1T + \frac{a_2}{2}T^2 + \frac{a_3}{3}T^3 + \frac{a_4}{4}T^4 + \frac{a_5}{5}T^5 + a_6\right) \quad (5-72)$$

$$s_i = R_g\left(a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7\right) \quad (5-73)$$

Here:

- $C_{p,i}$ (SI unit: J/(mol·K)) denotes the species' molar heat capacity,

- T (SI unit: K) is the temperature,
- R_g the ideal gas constant, 8.314 J/(mol·K),
- h_i (SI unit: J/mol) is the species' molar enthalpy, and
- s_i (SI unit: J/(mol·K)) represents its molar entropy at standard state.

From the CHEMKIN files the coefficients a_1 to a_7 are directly imported into the corresponding NASA format fields. Coefficients for NASA polynomials are available as public resources ([Ref. 11](#)).

Kinetics CHEMKIN files that can be imported in the [Reversible Reaction Group](#) feature. These consist of reaction kinetics data, such as activation energy (SI unit: J/mol).



Homogeneous Charge Compression Ignition of Methane: Application Library path **Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/compression_ignition**

Chemical Vapor Deposition of GaAs: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/gaas_cvd**

Working with Predefined Expressions

You can choose whether to use the predefined expressions as given, use parts of a predefined set of expressions, or replace expressions entirely. A few short examples highlight the use of the predefined expressions used in the [Transport Expressions](#) and [Thermodynamic Expressions](#) sections to enter the thermodynamic properties of carbon monoxide. The sections also illustrate the possibility to adapt to different modeling situations.

CASE I

Carbon monoxide is part of a reacting mixture. You want to do several things: make use of the predefined expressions of species C_p as an input to the heat capacity of the reacting mixture ([Equation 5-71](#)); use the predefined expression h for each species to calculate the heat of reaction ([Equation 5-72](#)); and use the predefined expression s for each species to calculate the entropy of reaction ([Equation 5-73](#)) and subsequently the equilibrium constant of reaction (See [Handling of Equilibrium Reactions](#)).

To accomplish this, enter the seven coefficients of the NASA format, a_1 to a_7 , into the appropriate fields, or import a [CHEMKIN Import for Species Properties](#) thermo input file.

CASE 2

Carbon monoxide is part of a reacting mixture. You want to make use of the predefined expressions of species C_p to calculate the heat capacity of the reacting mixture ([Equation 2-98](#)).

Polynomials for C_p are available in the literature ([Ref. 2](#), [Ref. 3](#), and [Ref. 5](#)) in the frequently used form

$$C_p = R_g \sum_n a_n T^{n-1} \quad n = 1, \dots, 5$$

You can directly use the predefined expression for the species' heat capacity, [Equation 5-71](#), also given in the C_p field, by supplying coefficients in the a_1 to a_5 fields.

You also want to use the predefined expressions h for each species to calculate the heat of reaction ([Equation 5-72](#)). An option is to make use of the heat of formation at standard state (298.15 K) to calculate the coefficient a_6 . Identifying the coefficient a_6 of [Equation 5-72](#) is straightforward. In the NASA polynomial format, the species molar enthalpy is related to its heat capacity according to

$$h = \int_0^T C_p dT + h(0) \quad (5-74)$$

Inserting [Equation 5-71](#) into [Equation 5-74](#), and comparing the result with [Equation 5-72](#), shows that the term $a_6 R_g$ is identified as the species enthalpy of formation at 0 K, that is, $h(0)$. Evaluate $h(0)$ from the species enthalpy of formation at standard state temperature, $T_{std} = 298.15$ K, which is given by

$$a_6 = \frac{h(T_{std})}{R_g} - \left(a_1 T_{std} + \frac{a_2}{2} T_{std}^2 + \frac{a_3}{3} T_{std}^3 + \frac{a_4}{4} T_{std}^4 + \frac{a_5}{5} T_{std}^5 \right) \quad (5-75)$$

CASE 3



Carbon monoxide is again part of a reacting mixture. It is satisfactory to approximate C_p as being constant. Specify the species enthalpy by making use of the heat of formation at 298 K, $h(298)$, according to the well-known expression

$$h = C_p(T - 298 \text{ K}) + h(298 \text{ K})$$

References for the Reaction Engineering Interface

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7. R.S. Brokaw, "Predicting Transport Properties of Dilute Gases," *Ind. Eng. Process Design Develop.*, vol. 8, no. 2, pp. 240–253, 1969.
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9. C. R. Wilke, "A Viscosity Equation for Gas Mixtures," *J. Chem. Phys.*, vol. 18, no. 4, pp. 517–519, 1950.
10. L.I. Stiel and G. Thodos, "The Viscosity of Polar Substances in the Dense Gaseous and Liquid Regions," *AIChE J.*, vol. 10, p. 26–29, 1964.
11. See, for example, www.comsol.com/chemical-reaction-engineering-module

The Reaction Engineering Interface

The **Reaction Engineering (re)** interface (), found under the **Chemical Species Transport** branch () when adding a physics interface, is used to model several chemical reactor types and the evolution of chemical reactions over time. The mass balance and energy balance equations describing these systems assume perfect or well-defined mixing in the reactor. Essentially, the physics interface simulates, tank, and plug flow chemical reactors to investigate the behavior over time of a chemical reaction.

The reaction kinetics expressions of a reactor can be exported to a space-dependent model, using the [Generate Space-Dependent Model](#) feature. This gives you the power to simulate reacting systems as they depend on fluid flow, mass transfer, and heat transfer — in other words, including space dependencies.

Add physics features from the toolbar, or right-click **Reaction Engineering** to select features from the context menu. Many of the fields and nodes described in this section are made available when either a [Reaction](#) or a [Species](#) (or both) subnode is added to the Model Builder. Because nodes and subnodes are accessible at any time, and any change is updated throughout the model, reactions and species are often defined before the settings described in this section.

All predefined constants and expressions can be overwritten by user-defined expressions. This makes it possible to go beyond the modeling assumptions that are the defaults in this physics interface.



- [Theory for the Reaction Engineering and Chemistry Interfaces](#)
- [Features Nodes Available for the Reaction Engineering Interface](#)

The following is a description of the features and fields available in the **Settings** window for Reaction Engineering.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to

different physics interfaces, the **name** string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model setup) is **re**.

EQUATION

This section displays the governing equations according to the selection of reactor types in the **Reactor** section.

REACTOR

Select a **Reactor type** to define the reaction system. The available reactor types are: **Batch**, **Batch, constant volume**, **CSTR**, **constant volume**, **CSTR, constant mass/generic**, **Semibatch**, and **Plug flow**. Each reactor type solves a mass balance based on properties typical to the type, such as reactor volume, volumetric production, or flow rate:

- **Batch**: In reactors no mass enters or leaves the system. This type can account for a variable reactor volume.
- **Batch, Constant Volume**: Same as Batch but where the reactor volume is assumed to be constant. As this is the situation for most reacting systems, this is the default condition.
- **CSTR, Constant Mass/Generic**: Continuous stirred tank reactors (CSTR) differ from batch reactors, since these allow species to enter and leave the reactor by means of feed inlet streams and outlet streams. The system's volume is allowed to change, such as in a car engine cylinder or a balloon. This reactor model can be solved either for a constant mass condition or by selecting a specific outlet flow.
- **CSTR, Constant Volume**: Same as the CSTR with constant mass/generic reactor but assumes that the volume is constant during operation.
- **Semibatch**: Semibatch reactors differ from batch reactors in that they allow reactants to enter the reactor by means of one or several feed inlet streams.
- **Plug Flow**: In the plug flow reactor, the species concentrations and the temperature vary with position. Plug flow in a tubular configuration means that concentration and temperature gradients develop only in the axial direction, but not in the radial direction.

For each **Reactor type**, additional settings are shown in [Table 5-1](#). If a surface reaction or species is included, except for the **Plug flow** reactor type, the surface reaction area is

also a parameter. The parameters and expressions are used in the mass balance equations.

TABLE 5-1: REACTOR TYPE PARAMETERS.

REACTOR TYPE	PARAMETERS TO DEFINE
Batch	Reactor volume V_r
Batch, constant volume	Reactor volume V_r
CSTR, constant mass/ generic	Volumetric production rate v_p and Volumetric outlet rate v
CSTR, constant volume	Volumetric production rate v_p and Reactor volume V_r
Semibatch	Volumetric production rate v_p
Plug flow	Volumetric flow rate v

Volumetric Rate

For **CSTR**, **constant volume** and **Semibatch** reactor types, the **Volumetric production rate** (v_p) is available. For **Automatic**, the in-built **Volumetric production rate** expression is shown. If **User defined** is selected, the expression can be changed (SI unit: m^3/s). For instance, this enables the setting of zero (0) volumetric production rate, which ignores volume changes due to reactions.

- For liquid phase reactions, the **Automatic** expression for the **Volumetric production rate** varies with the reaction rate of each species as defined by:

$$v_p = V_r \sum_i \frac{R_i M_i}{\rho_i}, \quad R_i = \sum_j v_{ij} r_j \quad (5-76)$$

The physics interface automatically inserts the stoichiometric coefficients (v_{ij}) and reaction rate expressions for each species (R_i) that depend on j number of reactions of a rate (r_j), as defined in the **Reaction** feature node. Furthermore, the values of the molar mass (M_i) and the species density (ρ_i) are automatically taken from the **Species** features.

- For gas phase reactions, the **Automatic** expression for the **Volumetric production rate** is similarly given by:

$$v_p = \frac{R_g T}{p} V_r \sum_i R_i, \quad R_i = \sum_j v_{ij} r_j \quad (5-77)$$

For **CSTR**, **constant mass/generic**, select **Volumetric rate** to either **Constant mass (Automatic)** or **Generic**. The **Constant mass (Automatic)** selection shows both the expression for **Volumetric production rate** (v_p) ([Equation 5-77](#) for gas, or

Equation 5-76 for liquid phase reactions) and **Volumetric outlet rate** (v) (Equation 5-78). The latter is derived from constant mass flow condition through the reactor:

$$v = \frac{\sum v_{f,m} \cdot \rho_{f,m}}{\rho} \quad (5-78)$$

The mixture density (ρ_f) of m number of feed inlet streams is determined in the same way as in the **Mixture Properties** section. For **Generic** both the **Volumetric rate** properties can be edited (SI unit: m^3/s). This means that it is possible to completely control the volumetric outlet rate from the CSTR.

For the **Plug flow** reactor, the **Volumetric flow rate** along the reactor is set. The **Automatic** definition computes a variable volumetric flow rate that depends on the molar flow rate of each species (F_i).

- For liquid phase reactions, the expression is:

$$v = \sum_i \frac{F_i M_i}{\rho_i} \quad (5-79)$$

- and for gas phase reactions:

$$v = \frac{R_g T}{p} \sum_i F_i. \quad (5-80)$$

The default value for p (**Reactor pressure**) is 1 atm in Equation 5-81 and it is set in the **Mixture Properties** section.

Reactor Volume

This input field sets the **Reactor volume** V_r — that is, the fluid volume in which chemical reaction takes place. The **Batch** reactor type can account for a changing volume, thus a time-dependent volume expression can be entered here.

Surface Reaction Area

Once a surface reaction, or a surface species, has been added, for all reactor types except **Plug flow**, the **Surface reaction area** settings become visible. Here, the area of the

surface on which the surface reactions take place can be defined. The surface area can either be defined directly as a parameter, or by defining the **Surface area to volume ratio**.



ENERGY BALANCE

From the list select to **Exclude** or **Include** the energy balance, which in essence determines whether the system is solved for either isothermal or nonisothermal conditions, respectively. The latter introduces the temperature as a variable in the interface.

If **Exclude** is chosen, enter a **Temperature** T for the system.

It is possible to incorporate cooling or heating of the reactor. This is done in **External heating or cooling** (Q_{ext}). Enter a negative value to account for cooling or a positive one for heating (SI unit: W). Note that for the Plug Flow reactor type, the **External heating or cooling** (Q) is defined per reactor volume (SI unit: W/m³).

MIXTURE PROPERTIES

Thermodynamics

All property parameters and property functions required by the interface can be automatically created by coupling to a system added to the **Thermodynamics** node. To do so click the **Thermodynamics** checkbox and select an existing [Thermodynamic System](#).

The **Thermodynamics** checkbox is enabled except if:

- the [Thermodynamics](#) node, including one or more systems, is not added under **Global Definitions**, or
- no species are added in the **Reaction Engineering** interface, or
- a CHEMKIN file is imported in the **Reaction Engineering** interface.

Phase

Use the **Phase** list to specify the state of aggregation of the mixture.

Density

This setting is available when the **Calculate mixture properties** checkbox in the **Calculate Transport Properties** section has been selected.

Two settings are always available for the mixture **Density: Automatic** or **User defined**. The **Thermodynamics** options is available when the interface is coupled to a [Thermodynamic System](#), and all interface species has been matched to species in the system. In this case the density is defined by a function automatically added under the thermodynamic system coupled to.

The mixture density is transferred to physics interfaces set up by the [Generate Space-Dependent Model](#) feature. The density is compiled for both multicomponent and solute-solvent solutions.

The **Automatic** setting uses the following logic:

- **Automatic** selected for **Liquid**, considers the liquid as ideal and incompressible. The liquid mixture density depends on the density of i number of pure species (ρ_i) and the species mass fraction (w_i).

$$\rho = \frac{1}{\sum_i \frac{w_i}{\rho_i}}$$

The mass fraction is given by the species concentration (c_i) and the molar mass (M_i).

$$w_i = \frac{c_i M_i}{\sum_i c_i M_i}$$

- **Automatic** set for **Gas** calculates the gas mixture density (ρ) from the concentrations (c_i) and molar masses (M_i) of the mixture species, which are automatically taken from [Species](#) features.

$$\rho = \sum_i c_i M_i \quad (5-81)$$

- If a [Type](#) is set to **Solvent** and the **Mixture** is **Liquid**, the mixture density is the same as the solvent density as defined in **Density** in **General parameters** in the Species node. When **Mixture** is **Gas**, the mixture density is calculated from [Equation 5-81](#) only for the species set as **Solvent**.

Reactor Pressure

The **Phase - Gas** setting displays the **Reactor pressure**. For all reactor types, except the **Plug flow** reactor, select either a pressure computed from the **Ideal gas law** or from any

other expression using the **User defined** option. The **Batch** and **Semibatch** reactor types also have the option to keep the reactor pressure **Constant** during reaction.

For the **Plug Flow** reactor, the **Reactor pressure** can be entered in the case of the **Reactor** section having the **Volumetric rate** set to **Automatic**, in which case the **User defined** alternative is available and a constant pressure fits the conditions.

When the **Thermodynamics** checkbox is selected in the **Mixture Properties** section and the species are fully coupled (see the section below), the reactor pressure is set to **Thermodynamics** indicating that it is automatically computed.

SPECIES MATCHING

The **Species Matching** section is activated when the **Thermodynamics** checkbox is selected in the **Mixture Properties** section. The species in the Reaction Engineering interface can be matched to species in the **Thermodynamic System**. This ensures that the arguments in the thermodynamic system functions are correctly defined.

Use the drop-down lists in the **From Thermodynamics** column to match each species in the interface to a species in the coupled thermodynamic system.

For each species matched, the required property parameters and functions are added under to the corresponding thermodynamic system.

When all species are matched, the interface is considered fully coupled and functions representing mixture properties, such as density, are also added automatically under the corresponding thermodynamic system.

CALCULATE TRANSPORT PROPERTIES

Transport properties are not utilized in the reactor equations available in the Reaction Engineering interface, where perfect mixing is assumed. However, transport properties such as diffusivity, thermal conductivity, and viscosity are of central importance when solving time- and space-dependent models. The physics interface helps to set up detailed expressions of species transport properties and transfers them automatically to the multiphysics model through the **Generate Space-Dependent Model** feature.

The most general description of a mixture is the one that treats the mixture as a multicomponent solution, where all species interact with each other. A simplified description, but still a common one, assumes that the solution has a solvent that dominates the properties of the solution. The solutes in such a solution interact only with solvent molecules.

Select the **Calculate mixture properties** checkbox to enable calculation of mixture transport properties exported from the Reaction Engineering interface.

From the list for each property, select the in-built **Automatic** expression or set a **User defined** entry. The mixture properties you can transfer for space-dependent models are:

- **Heat capacity** (c_p) (SI unit: J/(kg·K)) (this is available when the **Energy Balance** is set to **Include**)
- **Thermal conductivity** (k) (SI unit: W/(m·K))
- **Dynamic viscosity** (μ) (SI unit: Pa·s) (this is available when a **Type** is set to **Solvent**)
- **Mixture density** (ρ) (SI unit: kg/m³) (this is available in the **Mixture Properties** section)

All species properties needed to compute the mixture properties are entered in the **Species Transport Expression** or **Species Thermodynamic Expression** in the **Species** node.



Transport Expressions

EQUILIBRIUM SPECIES VECTOR

This section is available when at least one equilibrium reaction has been defined, that is, when a **Reaction** node incorporates at least one **Equilibrium** reaction (**Reaction type** is set to **Equilibrium**), or when at least one equilibrium reaction has been defined in an **Equilibrium Reaction Group**.

In the **Predefined dependent species (separated by ‘,’)** text field, edit, if necessary, the species that depends on the composition of the other species according to the **Equilibrium expression** in the **Reaction** node. To minimize the impact of any numerical errors, it is recommended to set the species with the highest concentration as dependent species. The default species is set to the leftmost species in the **Reaction formula**.

The **Suppress negative concentrations** checkbox exists to aid the computation of equilibrium reaction systems. A selected checkbox ensures that no negative values of concentrations are accepted as solution to the equilibrium condition.



Example II in Handling of Equilibrium Reactions.

ACTIVITY

Select the **Use activity** checkbox to solve for species activities instead of species concentrations, which is a common approach when nonideal fluids are modeled.

An activity coefficient other than 1 can be set for each species for the [Species](#) node in the **Species Concentration/Activity** section.



[Activity](#)

CHEMKIN IMPORT FOR SPECIES PROPERTIES


This section enables CHEMKIN[®] import to simulate complex chemical reactions in gas phase.

Two types of CHEMKIN input files can be imported here — **Thermo** and **Transport**, for thermodynamic properties and transport properties respectively. Properties for either volumetric or surface species are supported. Click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. For Thermo the imported data is directly entered in the **NASA format** fields in the [Species Thermodynamic Expressions](#) section. For Transport the imported data is entered in the [Species Transport Expressions](#) section.



- [CHEMKIN Data and NASA Polynomials](#)
 - [Reversible Reaction Group](#)
-

ADVANCED SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options**.

The **Uniform scaling of concentration variables** checkbox is not selected by default. When selected, all concentration variables are scaled using the same scale factor in the **Study** node. Enabling uniform scaling can decrease solver time for problems involving many concentration variables.

Features Nodes Available for the Reaction Engineering Interface

The following feature nodes are available from the **Reaction Engineering** ribbon toolbar (Windows users), **Reaction Engineering** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- [Initial Values](#)
- [Reaction](#)
- [Species](#)
- [Reversible Reaction Group](#)
- [Equilibrium Reaction Group](#)
- [Species Group](#)¹
- [Additional Source](#)
- [Reaction Thermodynamics](#)¹
- [Species Activity](#)²
- [Species Thermodynamics](#)¹
- [Feed Inlet](#)
- [Generate Space-Dependent Model](#)

¹ This node is always coupled to reaction group nodes and not available from context menu.

² This is a subnode and it is only available together with a parent node.

Initial Values

The **Initial Values** node sets the initial values of the dependent variables solved for in the Reaction Engineering interface.

GENERAL PARAMETERS

For **CSTR**, **constant mass** and **Semi** reactor types, in which the reactor volume changes with reaction, an **Initial system volume** V_{r0} can be set.

For nonisothermal conditions (that is, the [Energy Balance](#) is set to **Include**), enter an **Initial temperature** T_0 for the system. For the **Plug flow** reactor a corresponding **Inlet temperature** $T_{0,in}$ is entered.

VOLUMETRIC SPECIES INITIAL VALUES

In the **Volumetric Species Initial Values** table, the **Species** column automatically includes all the species in the model. Enter the corresponding values or expression for each species initially in the **Concentration (mol/m³)** column.

For the **Plug flow** reactor an **Inlet molar flow rate** table is instead shown. Enter the values or expressions representing the inlet conditions of each species in the **Molar flow rate (mol/s)** column.

SURFACE SPECIES INITIAL VALUES

The **Surface Species Initial Values** table is displayed when surface species are present in the reactor, that is, when the **Type** is set to **Surface species** for at least one species in the reactor. In the **Surface concentration (mol/m²)** column, enter the corresponding values or expression for each species initially on the reactive surface area (A_r) within the reactor. The values in the **Site occupancy number** column are by default set to 1, edit the value if a surface species takes up more than one active site on the reactive surface.


The total surface concentration is restricted by the molar amount of available sites on the reactive surface area. This is defined by the **Density of sites** Γ_s (mol/m²) entry. Make sure that the sum of the entered initial surface concentrations do not surpass the value selected here. Note that the total amount of sites occupied of a surface species $c_{ads,i}$ is the **Surface concentration (mol/m²)** multiplied with the **Site occupancy number** $\sigma_{s,i}$. The restriction of the total surface concentration is defined as:

$$\Gamma_s \geq \sum_i c_{ads,i} \sigma_{s,i} \quad (5-82)$$

EQUILIBRIA

When one or more equilibrium reactions are present, a section which allows the user to enable **Mass-preserving initialization** is shown. When enabled, the solver will first solve for the values of the species participating in any equilibrium reaction, while disregarding any kinetic reactions. The solution to the equilibrium subproblem is then used as a consistent starting point for the time stepping. The functionality solves a log-transformed version of the problem, which in turn puts a requirement that a finite concentration is present for each building block (atom kinds, charge, and/or a combination thereof). If **Settings** is changed from **Automatic** to **Manual**, the user may change the maximum number of iterations and the absolute tolerance.

Reaction

Use the **Reaction** node () to implement a chemical reaction involving a number of chemical species. The participating species may represent any kind of molecular entities like atoms, molecules, ions, or radicals.

To add a **Reaction** node either right-click the **Reaction Engineering** node or on the **Reaction Engineering** toolbar click **Reaction**.

REACTION FORMULA

Formula

Enter a chemical equation in the **Formula** field. The chemical equation should be of the format “A + B \rightarrow C + D”. Here, A and B are reactants, C and D are product species, and \rightarrow denotes a reaction arrow. The participating species should be written with [Valid Species Names](#). Valid reaction arrows are “ \rightleftharpoons ” for reversible reaction, “ \Rightarrow ” for irreversible reaction, and “ \equiv ” for equilibrium reaction. Species can be given trivial names, or their chemical formulas can be used as names. Examples of valid formulas are; “carbon+oxygen \Rightarrow carbondioxide”, and “C(s)+O₂(g) \Rightarrow CO₂(g)”.

Click **Apply** to let the interface parse the reaction. This process identifies the participating species as well its stoichiometric coefficients and any charges of ionic species. A [Species](#) feature is automatically added for all participating species.

Balance

Use the **Balance** button to automatically calculate the stoichiometric coefficients such that the number of atoms of each kind are the same on both sides of the reaction. This turns, for example, the formula “H₂+O₂ \Rightarrow H₂O” into “2H₂+O₂ \Rightarrow 2H₂O”. The balancing involves parsing all participating species for elements in the periodic table. It therefore requires that all species in the **Formula** field are written either using their chemical formula, say “H₂O”, or that each species in the reaction have an enabled **Chemical Formula** field in their **Species** node. For example, it is possible to balance the formula “H₂+O₂ \Rightarrow water” as long as there is a Species node with the name “water” already present, and an enabled **Chemical Formula**.

For automatic reaction balancing to be successful, requires that the problem is well posed. One example of a problem that is not well posed is “C+H₂ \Rightarrow CH₄+C₂H₆”, in which case any ratio of CH₄/C₂H₆ could be obtained. Another example is “H₂ \Rightarrow O₂” where not all elements are present on both sides.

Reaction Type

Select the **Reaction type** — **Reversible**, **Irreversible**, or **Equilibrium** — or edit the expression directly in the **Formula** field. In the latter case, specify the reaction type with a delimiter separating the two sides of the equation:

- \rightleftharpoons denotes a **Reversible** reaction
- \Rightarrow denotes an **Irreversible** reaction
- \equiv denotes a reaction at chemical **Equilibrium**

Each **Reaction type** has its own set of reaction kinetics:

- When the reaction is **Reversible** or **Irreversible**, the rate of reaction r_j , for reaction j , contributes to the change in species i in the manner of:

$$R_i = \sum_j \nu_{ij} r_j \quad (5-83)$$

where ν_{ij} is the stoichiometric coefficient.

- In the case of an **Equilibrium** reaction, the equilibrium expression is equal to the equilibrium constant:

$$K_{eq} = K_{eq0} \quad (5-84)$$

REACTION RATE

This section is available when the **Reaction type** is either **Reversible** or **Irreversible**.

When **Mass action law** is selected (default), the rate expression is automatically derived from the stoichiometric coefficients in the reaction formula:

- For an **Irreversible** reaction type, the reaction rate becomes:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} \quad (5-85)$$

- For a **Reversible** reaction type, the expression instead becomes:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}} \quad (5-86)$$

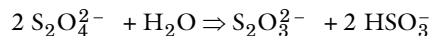
The deduced overall reaction order is shown in text below the respective equation in the **Reaction Rate** section.

Arbitrary rate expression

If the reaction order differs from the stoichiometric coefficients, or if an arbitrary rate expressions is applicable, change **Reaction Rate** to **User defined**. An expression field r appears with the default expression being that from the mass action law. Below this there are fields to set the reaction order. For a reversible reaction the reverse reaction order may be specified in addition to the forward one. The unit of the rate constant k (or frequency factor A in the case of Arrhenius behavior), is derived from the reaction order, in SI units: $(\text{m}^3/\text{mol})^{\alpha-1}/\text{s}$, where α equals the order with respect to volumetric species. When surface species are present — identified by their “(ads)”

suffix — the unit is instead given by $\text{m}^{3\alpha+2\beta-2}/\text{mol}^{\alpha+\beta-1}/\text{s}$, where β is the order with respect to surface species.

Consider for example the reaction:



The automatically deduced reaction order is three, however, in the case that water is the solvent, the order should probably be two. This is specified as follows:

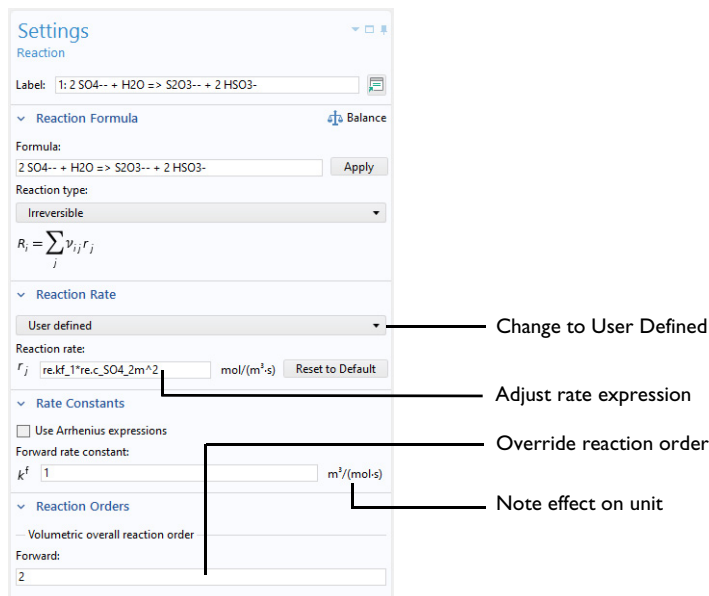


Figure 5-5: The reaction order can be manually specified for a user defined reaction rate.

RATE CONSTANTS

This section applies for **Reversible** or **Irreversible** reactions and defines the reaction rate constants used in the reaction rates.

Forward Rate Constant and Reverse Rate Constant

The **Forward rate constant** k^f is used for both **Reversible** and **Irreversible** reactions. The **Reverse rate constant** k^r is only used for **Reversible** reactions (Equation 5-86).

The SI units of the rate constants are automatically based on the order of the reaction with respect to the concentrations, as defined in the **Reaction formula**.

Specify Equilibrium Constant

The **Specify equilibrium constant** checkbox is available for **Reversible** reactions. If the checkbox is selected the rate constants are defined in a different manner with the reverse rate constant being computed from the following expression:

$$k^r = k^f / K_{eq0} \quad (5-87)$$

Thus, in this case, the forward rate constant and equilibrium constant for the reaction are needed. The **Equilibrium constant** is edited in the [Equilibrium Settings](#) section.

Use Arrhenius Expressions

When the **Use Arrhenius expressions** checkbox is selected the Arrhenius parameters are automatically used in predefined expressions for the forward and reverse rate constants k^f and k^r , respectively.

$$k^f = A^f (T/T_{ref})^{n^f} \exp(-E^f/(R_g T)) \quad (5-88)$$

$$k^r = A^r (T/T_{ref})^{n^r} \exp(-E^r/(R_g T)) \quad (5-89)$$

Specify the activation energy and the frequency factor in the Arrhenius expressions to account for temperature variations. The reference temperature, T_{ref} equals 1 K. The available fields are based on the **Reaction type** chosen in the [Reaction](#) node. Enter values or expressions for each of the following (reverse expressions are only available for reversible reactions):

- **Forward frequency factor** A^f and **Reverse frequency factor** A^r (unit depends on reaction order)
- **Forward temperature exponent** n^f and **Reverse temperature exponent** n^r
- **Forward activation energy** E^f and **Reverse activation energy** E^r (SI unit: J/mol)

EQUILIBRIUM SETTINGS

This section is available for equilibrium reactions, and for reversible reactions when the **Specify equilibrium constant** checkbox has been selected.

Equilibrium Expression

For an equilibrium reaction, specify the **Equilibrium expression**. When the **Equilibrium expression** is set to **Automatic** the following expression is used:

$$K_{eqj} = \frac{\prod_{i \in \text{prod}} c_i^{v_{ij}}}{\prod_{i \in \text{react}} c_i^{-v_{ij}}} \quad (5-90)$$

Select **User defined** from the **Equilibrium expression** list to instead enter a manually defined equilibrium expression.

Equilibrium Constant

Specify the **Equilibrium constant** K_{eq0} for an equilibrium reaction, or for a reversible reaction when the **Specify equilibrium constant** checkbox has been selected (in the **Rate Constants** section).

The **Equilibrium constant** can either be **User defined**, or automatically defined when set to **Automatic** or **Thermodynamics**.

Use the **Automatic** option to compute the equilibrium constant for an ideal system. This setting requires that the temperature is also solved for by setting **Energy Balance** to **Included**.

The **Thermodynamics** option is available when all reactions in the interface are equilibrium reactions, and the interface is fully coupled to a **Thermodynamic System** (see **Species Matching**). Use this setting to automatically compute the equilibrium constant for an ideal or nonideal system, dependent on the thermodynamic model applied for the coupled system.

Using **Automatic** or **Thermodynamics**, K_{eq0} is calculated from the Gibbs free energy of the reaction. For more details see **The Equilibrium Constant** and the **Automatically Defined Equilibrium Constants** section therein.

REACTION THERMODYNAMIC PROPERTIES

This section contains information about thermodynamic properties that relate to a selected reaction and is available when the **Energy Balance** is set to **Include**. Several **Automatic** definitions are available here.

Enthalpy of Reaction

The **Enthalpy of reaction** H (SI unit: J/mol) is calculated by the interface from species properties and the related stoichiometric coefficients:

$$H_j = \sum_{i \in \text{prod}} v_{ij} h_i - \sum_{i \in \text{react}} (-v_{ij}) h_i \quad (5-91)$$

Entropy of Reaction

The **Entropy of reaction** S (SI unit: J/(mol·K)) comes from a similar expression:

$$S_j = \sum_{i \in \text{prod}} \nu_{ij} s_i - \sum_{i \in \text{react}} (-\nu_{ij}) s_i \quad (5-92)$$

In [Equation 5-91](#) and [Equation 5-92](#), h_i and s_i are the species' molar enthalpy and molar entropy, respectively.

Enter these quantities in the **Thermodynamic Expressions** section for the [Species](#) node either by using the predefined polynomial or by providing a custom expression or constants.

The stoichiometric coefficients ν_{ij} , are defined as being negative for reactants and positive for products. Using [Equation 5-91](#) and [Equation 5-92](#) to equate the Gibbs free energy of reaction enables the equilibrium constant to be expressed according to [Handling of Equilibrium Reactions](#).

Heat Source of Reaction


The **Heat source of reaction** (SI unit: W/m³) is automatically computed from the heat of each reaction j , given by:

$$Q_j = -r_j H_j$$



Using the Reaction Node

Species

When a [Reaction](#) is defined, a **Species** node () is automatically generated for the participating reactants and products. This feature enables you to review and enter species specific information regarding chemical kinetics, thermodynamics, and transport properties.

It is also possible to add and define an individual **Species** node: on the **Reaction Engineering** toolbar click **Species** or right-click the **Reaction Engineering** node and select it from the context menu.

NAME

When a **Species** node is automatically generated using the **Formula** text field in the **Reaction** node, the species name is also automatically generated.

For a **Species** node added individually, enter a **Name** in the field and click **Apply**. By entering a name consisting of only elements from the periodic table, the chemical formula is added, and molar mass is calculated and added in the **Chemical Formula** section. The species charge, and type, are also deduced from the species name.



Valid Species Names

TYPE

Select a species type — **Bulk species**, **Surface species**, or **Solvent**.

Bulk species are solved for volumetric concentrations (SI unit: mol/m^3), while **Surface species** are solved for surface concentration (SI unit: mol/m^2). The compositions for **Bulk species** and **Solvent** (not solved for) use the syntax `c_speciesname`, while **Surface species** uses `csurf_speciesname_surf`.

Surface species is referring to species adsorbed on a reactive surface. When **Surface species** is selected, the corresponding reaction formula introduces (**ads**) after the species notation and changes the species' name to `speciesname_surf`. Additionally, the Species node name is updated in a similar fashion.

For the **Plug flow** reactor only **Bulk species** and **Solvent** are allowed.



Choosing the Species Type

CHEMICAL FORMULA

The **Chemical Formula** section contains the species chemical formula, **Molar mass**, M , and **Charge**, z .

If the name entered for the species consists of only elements from the periodic table, and optionally charge and phase indication, then the **Chemical Formula** field will be populated with the name entered in the **Name** section, and the molar mass and charge will be added to this section. The species molar mass is computed from the mass of

occurring individual elements¹. The rules for writing chemical formulas are the same as those for **Species** names.



Valid Species Names

When the species name contains parts not in the periodic table, for example when a descriptive name such as **water** is used, the molar mass is set to 0.0 kg/mol. If the species name consists of a valid charge or phase indication, then charge and type will be set automatically. In this case, the molar mass needs to be defined in order to achieve mass balanced reactions and correct definitions of mass basis properties. By entering a chemical formula consisting only of elements from the periodic table (and optionally charge and phase indication), the molar mass, and charge are derived automatically.

When needed, the **Molar mass** can be edited in the corresponding text field. Editing the **Chemical formula** and pressing apply will override the content in the molar mass and charge fields. The **Charge** field cannot be edited as long as a chemical formula is enabled.

With an enabled **Chemical Formula** it is possible to use the trivial name of a species and balance reactions. Having added the Species **water**, **oxygen**, and **hydrogen**, and filled in H₂O, O, and H in their respective chemical formula sections, the **Formula** oxygen+hydrogen=water is balanced into oxygen+2hydrogen=water by clicking **Balance** in the **Reaction** node.

It is possible to specify the species density ρ when the fluid **Mixture** is specified as **Liquid**. The default value is that of water at 293 K.

REACTION RATE

Change the **Automatic** default setting to **User defined** to use a species reaction rate other than the one set up in the associated **Reaction** node. For individual species, use the **User defined** option to set a reaction rate other than zero (that is, nonreactive).

Edit either the **Rate expression** (SI unit: mol/(m³·s)), the **Surface rate expression** (SI unit: mol/(m²·s)), or both. For a bulk species, both expressions appear if surface reactions are present in the reactor since the reaction of the species can depend both on bulk reaction R and surface reaction R_{ads} rates. For a surface species, only the surface reaction rate R_{ads} appears.

1. Values are averages of upper and lower bounds for each atom as published by CIAAW. Source: CIAAW. Atomic weights of the elements 2019. Available online at www.ciaaw.org.

The reaction rate is not editable if the species in question participates in an equilibrium reaction and has been selected as a **Predefined dependent species** in [Equilibrium Species Vector](#).

CONSTANT CONCENTRATION/ACTIVITY

To account for nonideality in the fluid mixture adjust the activity coefficient in the **Activity coefficient** text field here. The section is only shown if activity instead of concentration has been chosen in the interface; that is, the **Use activities** checkbox is selected on the Reaction Engineering interface **Settings** window

Click to select the **Keep concentration/activity constant** checkbox if the species concentration or activity should be treated as constant.

TRANSPORT EXPRESSIONS

Here the required parameters to compute various transport properties can be edited. To show this section the **Calculate mixture properties** checkbox needs to be selected under the **Calculate Transport Properties** section in the **Settings** window of the physics interface.

- For a gas mixture, there are maximum five properties to consider:
 - σ , the characteristic length (unit: Å) of the Lennard–Jones/Stockmayer potential
 - ϵ/k_b (SI unit: K) the potential energy minimum value of the Lennard–Jones/Stockmayer potential, divided by Boltzmann’s constant. Tabulated data in the literature frequently lists values of ϵ/k_b rather than ϵ
 - μ_D , the dipole moment (SI unit: Debye)
 - k_i , the thermal conductivity of the gas (SI unit: W/(m·K)); and Diffusivity of the species (SI unit: m²/s). The latter two can be set to **Automatic**, when σ and ϵ/k_b have been given.
- For mixtures of gas with solvent, all properties above except the thermal conductivity is shown. This is instead calculated under the **Calculate Transport Properties** section in the Settings window for the Reaction Engineering interface. This requires that [Energy Balance](#) is set to **Included**.
- For a liquid mixture, there is only the parameter k_i , the thermal conductivity (SI unit: W/(m·K)) to edit.
- For mixtures of liquid with solvent, the thermal conductivity is shown only for the species set as **Solvent**.

THERMODYNAMIC EXPRESSIONS

The parameters utilized for calculation of thermodynamic mixture and reaction properties are set in this section. It is accessed when the [Energy Balance](#) is set to **Include** for the Reaction Engineering interface, in other words, for nonisothermal conditions.

The **Thermodynamic Expressions** are by default computed using data in the **NASA format**. In this case, enter the following to compute the species' heat capacity, C_p (SI unit: J/(mol·K)), the molar enthalpy, h (SI unit: J/mol), and the molar entropy, s (SI unit: J/(mol·K)):

- **Lower temperature limit** T_{lo}
- **Middle temperature limit** T_{mid}
- **Upper temperature limit** T_{hi}
- **Polynomial coefficients** $a_{low,k}$ and $a_{hi,k}$

Any coefficients for the thermodynamic polynomials entered into the $a_{low,k}$ fields apply to the temperatures in the range T_{lo} to T_{mid} ; coefficients entered into the $a_{hi,k}$ fields apply to temperatures in the range T_{mid} to T_{hi} range. The coefficients can also be imported in the **CHEMKIN Import for Species Properties** section in the Reaction Engineering node.


Choose the **User defined** alternative to specify C_p , h , and s directly.



[Using the Species Node](#)

[Transport Properties](#)

Reversible Reaction Group

The **Reversible Reaction Group** node () allows input of a large number of reversible reactions in the same table. All reactions are treated in the same way. More than one Reversible Reaction Group can be added to a component. The feature is typically used when importing CHEMKIN kinetics files.







Add the node from the **Reaction Engineering** toolbar or right-click **Reaction Engineering** and add it from the context menu.

For the case when reaction kinetics data are entered manually into the **Reaction table** and nonisothermal conditions apply ([Energy Balance](#) is set to **Include**), right-click to add a [Reaction Thermodynamics](#) subnode or select it from the **Reaction Engineering**

toolbar, **Attributes** menu. In it, the Enthalpy of Reaction (J/mol) for each reaction can be specified.

REACTION TABLE

The reversible reactions in the **Reaction table** are numbered and contain reactants, products, and kinetic parameters describing the reaction. Use the buttons under the **Reaction table** to add and sort the reaction details.

- In general, use the **Move Up** (), **Move Down** (), and **Delete** () buttons and the fields under tables to edit the table contents. Or right-click a table cell and select **Move Up**, **Move Down**, or **Delete**.
- The **Add** button () adds default reactant, A, and product, B, with a default. Click the corresponding field to edit the reactant, product, or parameters. After editing the **Species Group** node is also updated. It is created together with the reaction group.
- You can save the parameters to a text file to reuse in other models. Click the **Save to File** button () and enter a **File name** in the **Save to File** dialog, including the extension .txt. Click **Save** to store the parameters in a text file or in a Microsoft Excel Workbook spreadsheet if the license includes LiveLink™ for Excel®. The information is saved in space-separated columns in the same order as displayed on screen. When saving to Excel, an **Excel Save** dialog appears where you can specify the sheet and range and whether to overwrite existing data, include a header, or use a separate column for units.
- You can import or load data in files from a spreadsheet program, for example, with the **Load from File** button () and the **Load from File** dialog that appears. Data must be separated by spaces or tabs. If there is already data in the table, imported parameters are added after the last row. Move or edit rows as needed. If the license includes LiveLink™ for Excel® you can also load parameters from a Microsoft Excel Workbook spreadsheet. Then an **Excel Load** dialog appears where you can specify the sheet and range and whether to overwrite existing data. It is also possible to import from a spreadsheet containing a separate column for units.

CHEMKIN IMPORT FOR KINETICS

Click to select the **Import CHEMKIN data** checkbox to import a CHEMKIN **Kinetics input file**. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**.




CHEMKIN Data and NASA Polynomials

MOVE REACTION AND SPECIES

Enter a reaction number in the **Moving reaction (with the number) from table** text field and click **Create Reaction** to remove the reaction from the **Reaction table** to the model tree. This introduces a reaction node named after the reaction number and species names and simultaneously creates corresponding species nodes. This action is powerful, since it enables all the editing possibilities available for [Reaction](#) and [Species](#) nodes.

Equilibrium Reaction Group



The **Equilibrium Reaction Group** node () allows for input of a large number of equilibrium reactions in the same table. This node functions in the same way as the [Reversible Reaction Group](#) for reversible reactions.




Add the node from the **Reaction Engineering** toolbar or right-click **Reaction Engineering** and add it from the context menu.

For the case when reaction kinetics data are entered manually into the **Reaction table** and nonisothermal conditions apply ([Energy Balance](#) is set to **Include**), right-click to add a [Reaction Thermodynamics](#) subnode or select it from the **Reaction Engineering** toolbar, **Attributes** menu. In it, the Enthalpy of Reaction (J/mol) for each reaction can be specified.

EQUILIBRIUM REACTION TABLE

The equilibrium reactions in the **Reaction table** are numbered and contain reactants, products, and equilibrium constants. Use the buttons under the **Reaction table** to add and sort the reaction details.

- In general, use the **Move Up** (), **Move Down** (), and **Delete** () buttons and the fields under tables to edit the table contents. Or right-click a table cell and select **Move Up**, **Move Down**, or **Delete**.

- The **Add** button () adds default reactant, A, and product, B, with a default. Click the corresponding field to edit the reactant, product, or parameters. After editing the **Species Group** node is also updated. It is created together with the reaction group.
- You can save the parameters to a text file to reuse in other models. Click the **Save to File** button () and enter a **File name** in the **Save to File** dialog, including the extension .txt. Click **Save** to store the parameters in a text file or in a Microsoft Excel Workbook spreadsheet if the license includes LiveLink™ for Excel®. The information is saved in space-separated columns in the same order as displayed on screen. When saving to Excel, an **Excel Save** dialog appears where you can specify the sheet and range and whether to overwrite existing data, include a header, or use a separate column for units.
- You can import or load data in files from a spreadsheet program, for example, with the **Load from File** button () and the **Load from File** dialog that appears. Data must be separated by spaces or tabs. If there is already data in the table, imported parameters are added after the last row. Move or edit rows as needed. If the license includes LiveLink™ for Excel® you can also load parameters from a Microsoft Excel Workbook spreadsheet. Then an **Excel Load** dialog appears where you can specify the sheet and range and whether to overwrite existing data. It is also possible to import from a spreadsheet containing a separate column for units.

MOVE REACTION AND SPECIES


Enter a reaction number in the **Moving reaction (with the number) from table** text field and click **Create Reaction** to remove the reaction from the **Reaction table** to the model tree. This introduces a reaction node named after the reaction number and species names and simultaneously creates corresponding species nodes. This action is powerful, since it enables all the editing possibilities available for **Reaction** and **Species** nodes.



Homogeneous Charge Compression Ignition of Methane: Application Library path **Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/compression_ignition**

Chemical Vapor Deposition of GaAs: Application Library path **Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/gaas_cvd**

Species Group

The **Species Group** node () contains information on a molecular level about the volumetric species and the surface species present in the model. The **Property for Volumetric Species** or **Property for Surface Species** tables typically collect parameters from when importing CHEMKIN transport files.

This node is automatically created when either the [Reversible Reaction Group](#) or the [Equilibrium Reaction Group](#) is added. The created species group node is coupled to the corresponding reaction group feature. If a reaction group feature is removed, disabled or enabled, the coupled species group feature will follow the same actions. The species in species group feature are only from its corresponding reaction group feature.

For the case of nonisothermal reactor conditions ([Energy Balance](#) is set to **Include**), a [Species Thermodynamics](#) subnode is automatically created in which the thermodynamic properties of the species can be specified.


CHEMKIN

This section allows import of CHEMKIN transport files. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. Note that this section is only shown when transport properties are computed (**Calculate mixture properties** checkbox under the **Calculate Transport Properties** is selected).



[CHEMKIN Data and NASA Polynomials](#)

Additional Source

Use the **Additional Source** node () to add an additional rate expression (SI unit: mol/m^3) and/or an additional volumetric production rate (SI unit: m^3/s) to the mass balance of certain species.

Add the node from the **Reaction Engineering** toolbar or right-click **Reaction Engineering** and add it from the context menu.

ADDITIONAL VOLUMETRIC PRODUCTION RATE

An additional **Additional volumetric production rate** can be added for some of the available reactor types, namely **CSTR, constant mass/generic, CSTR, constant volume**, or **Semi**.


ADDITIONAL RATE EXPRESSION

Here, values or expressions describing additional rates can be entered for selected **Species** in the column denoted **Additional rate expression (mol/m³*s)** within the **Volumetric species** table.

ADDITIONAL SURFACE SPECIES RATE


Here, values or expressions describing additional surface species rates can be entered for selected **Surface species** in the column denoted **Additional rate expression (mol/m²*s)** within the **Surface species** table.

Reaction Thermodynamics

In the **Reaction Thermodynamics** subnode (), the Enthalpy of Reaction (SI unit: J/mol) of each reaction can be specified. This node overrides all the automatically calculated reaction enthalpies as defined in the [Species Thermodynamics](#) subnode.


Add the **Reaction Thermodynamics** node from the **Reaction Engineering** toolbar, **Attributes** menu. Alternatively, when the **Energy Balance** is set to **Include**, right-click a [Reversible Reaction Group](#) or [Equilibrium Reaction Group](#) and select it from the context menu.

Species Activity

The **Species Activity** subnode () creates variables for the activities for all the species/surface species present in the Species Group parent feature. Edit the **Activity coefficient** field in the **Species Activity** or **Surface Species Activity** tables by clicking in these.

Species Activity is a subnode to the [Species Group](#) node. It is automatically generated when nonideality in the fluid mixture is accounted for; when the **Use activity** checkbox is selected in the **Activity** section.

Species Thermodynamics

The **Species Thermodynamics** node () creates variables for the enthalpies, entropies, and heat capacities for all the species/surface species present in the [Species Group](#)

parent feature. The purpose is to compute thermodynamic mixture properties and the heat of reactions.

This node is a subnode to the [Species Group](#) node when the [Energy Balance](#) is set to **Include**.

THERMODYNAMICS PROPERTIES OF SPECIES

Select a **Type selection** for the thermodynamic properties. The **NASA format** alternative requires the setting of several polynomial constants and is typically used together with CHEMKIN import. The **User defined** alternative only requires input of Species molar enthalpy (SI unit: J/mol) and Species molar capacity (SI unit: J/(mol·K)).


CHEMKIN IMPORT FOR THERMODYNAMIC DATA

This section allows import of thermodynamic CHEMKIN transport files. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. Note that this can only be done for the **NASA format** option.



- [CHEMKIN Data and NASA Polynomials](#)
-

Feed Inlet

The **Feed Inlet** () feature is used for adding inlet streams to the reactor.

After adding a [Reaction](#) node and setting its [Reactor](#) to **CSTR**, **constant volume**, **CSTR**, **constant mass/generic**, or **Semi**, add a **Feed Inlet** node from the **Reaction Engineering** toolbar or right-click the **Reaction Engineering** node to add it from the context menu.

FEED INLET PROPERTIES

Edit the **Volumetric feed rate** (v_f) (SI unit: m³/s) to fit the modeling conditions.

The **Feed inlet temperature** (T_f) is required as input when nonisothermal conditions are investigated ([Energy Balance](#) is set to **Include**).

FEED INLET CONCENTRATION


This section is available when [Energy Balance](#) is set to **Exclude**.

For each of the Species, enter a value or expression in the table for the **Concentration** (mol/m³) to set the composition of the inlet stream.

FEED INLET CONCENTRATION AND ENTHALPY


This section is available when [Energy Balance](#) is set to **Include**.

For each of the Species, enter values or expressions in the table for the **Concentration (mol/m³)** and **Enthalpy (J/mol)** to set both the composition and enthalpy of the feed inlet stream. Note that in the rightmost column of the **Feed inlet concentration and enthalpy** table, it is possible to select that the thermodynamic properties are taken from a [Species](#) node instead.

	<ul style="list-style-type: none">• CSTR, Constant Mass/Generic• CSTR, Constant Volume• Semibatch
---	---

Generate Space-Dependent Model

It is often relevant to perform an extended analysis of the reaction model. For example, to study how a reacting system's detailed geometry impacts the concentration and temperature distributions. Use the **Generate Space-Dependent Model** feature to export the properties within the Reaction Engineering interface to physics interfaces solving for fluid flow, mass transport and heat transfer in a space-dependent geometry. Properties exported from Reaction Engineering are reaction kinetics, thermodynamics, and transport parameters. The reaction kinetics are replicated in a Chemistry interface added to the space-dependent component. The physicochemical properties in Chemistry can be coupled to mass, fluid and heat transfer interfaces.

To add the **Generate Space-Dependent Model** node, find the **Reaction Engineering** toolbar and click **Generate Space-Dependent Model** () or right-click the **Reaction Engineering** node to add it from the context menu. Note that only a single **Generate Space-Dependent Model** node can be added.

SELECTING THE GEOMETRY AND PHYSICS INTERFACES

When using the **Generate Space-Dependent Model** feature, select which geometry and physics interfaces to create in the following manner:

- 1 Select the component to use: 1D, 1D Axisymmetric, 2D, 2D Axisymmetric, 3D, or an existing component in the Model Builder.
- 2 Select the physics interfaces to use in each category (chemical species transport, fluid flow and heat transfer).
- 3 Select a study type.

Then click the **Create/Refresh** button at the top of the settings window (see [Figure 5-6](#)). A new Chemistry interface is generated by default when a new geometry or a new chemical species transport interface is selected. It is also possible to add a new Chemistry interface to an existing component, for example after changing the reaction mechanism, by using the **Chemistry** list and setting the other lists to **None**.

In the context of electric discharge simulations, it is recommended to use [The Transport of Charge Carriers Interface](#) as a chemical species transport interface. [The Transport of Charge Carriers Interface](#) closely resembles [The Transport of Diluted Species Interface](#). The primary distinction lies in its use of a logarithmic formulation, which enhances accuracy when the charge carrier density spans multiple orders of magnitude.

When possible, one or several multiphysics coupling features are automatically added under the Multiphysics node in the Model Builder window. The coupling node simplifies multiphysics models by synchronizing settings between interfaces. When for example a **Transport of Diluted Species** interface is created together with a **Laminar Flow** interface, a **Reacting Flow, Diluted Species** multiphysics coupling node is also added.

To add physics interfaces to an existing component, simply select the component from the **Components to use** list, use the **Physics Interfaces** section to select additional interfaces, and click the **Create/Refresh** button.

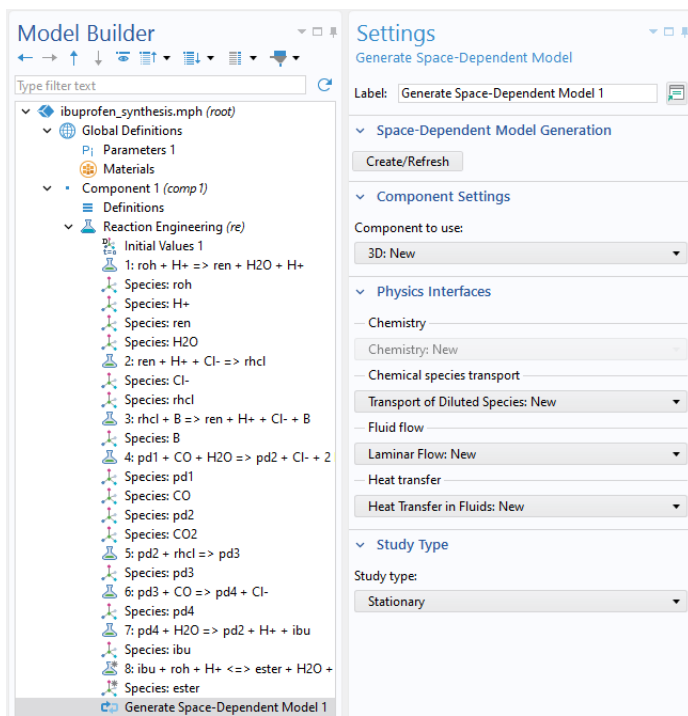


Figure 5-6: Using the Generate Space-Dependent Model node the reaction mechanism in a Reaction Engineering interface is transferred to physics interfaces in a space-dependent component (1D, 1D Axisymmetric, 2D, 2D Axisymmetric, or 3D).

COMPONENT SETTINGS

Select a **Component to use**. Either specify the space dimension of a new component — **1D**, **1Daxi**, **2D**, **2Daxi**, or **3D** — or select a component already present in the Model Builder. The geometry selection affects the content of other interface lists. For example, the reacting flow interfaces are only available in 2D and 3D.

PHYSICS INTERFACES

Select the applicable physics interfaces to create from the **Chemical species transport**, **Fluid flow**, and **Heat transfer** lists. The interfaces available depends on the reaction system. When a solvent species is defined, a diluted solution is assumed and available interfaces for mass transport are based on the **Transport of Diluted Species** interface. When no solvent is defined, interfaces based on **Transport of Concentrated Species** are also available.

The **Chemical species transport** list contains two categories of mass transfer interfaces, as seen in [Figure 5-7](#). The top of the list contains single physics interfaces, such as **Transport of Diluted Species**. These can be used together with other single physics interfaces, from the **Fluid Flow** or **Heat Transfer** lists, to create a manual multiphysics setup.

The **Chemical species transport** list also contains predefined multiphysics interfaces, like **Reacting Flow** or **Reacting Flow in Porous Media**. Selecting one of these automatically includes multiple interfaces, as well as dedicated coupling features. These multiphysics interfaces correspond to the ones available in the **Chemical Species Transport** branch of the Model Wizard or the Add Physics window. When different versions the interface exists, additional lists corresponding to sub-branches (in the Model Wizard) are enabled. An example of a multiphysics interface version is shown in [Figure 5-8](#), where the **Porous Catalyst, Transport of Concentrated Species** version of the **Reacting Flow in Porous Media** has been selected.

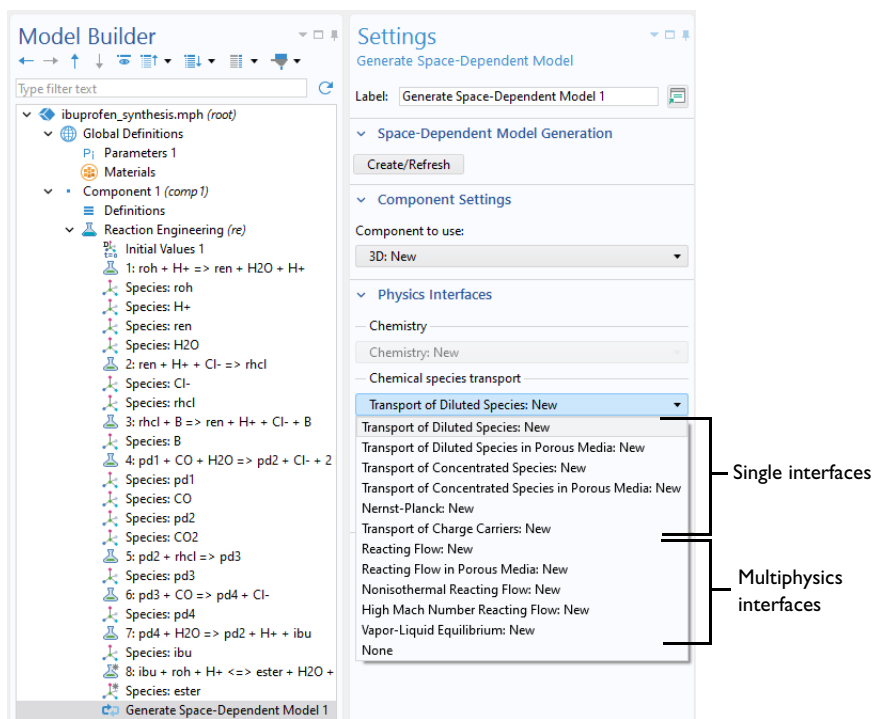


Figure 5-7: The Chemical species transport list contains both single interface entries as well as multiphysics interfaces.

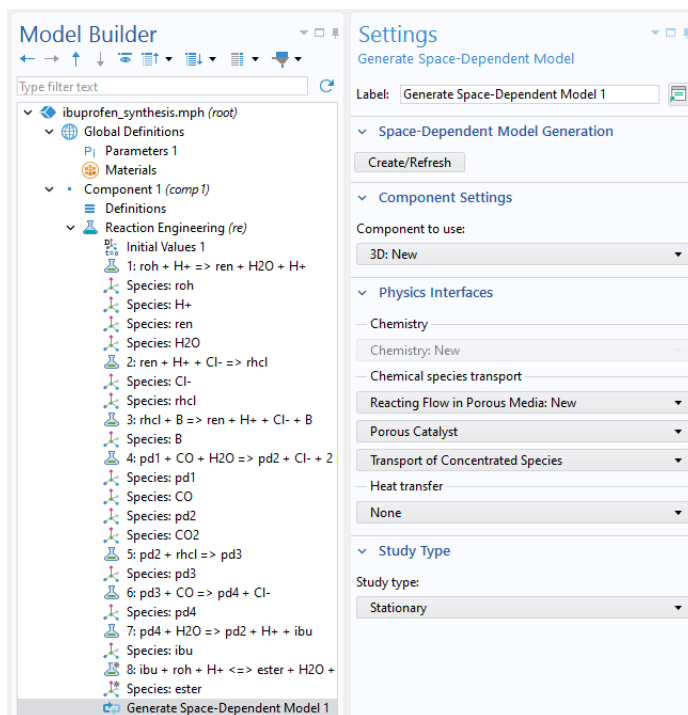


Figure 5-8: The Porous Catalyst, Transport of Concentrated Species version of the Reacting Flow in Porous Media interface is one example of a multiphysics interface that can be created from the Generate Space-Dependent Mode node.

The [Chemistry Interface](#) is always created and added when generating a new component or a new chemical species transfer interface. It generates global variables for the reaction kinetics, thermodynamics, and transport properties. The variables generated are available for all space-dependent interfaces. [Figure 5-9](#) displays an application where a Reactions feature uses reaction rates defined by a Chemistry interface. The syntax `chem` points to the default **Name** of the Chemistry node.

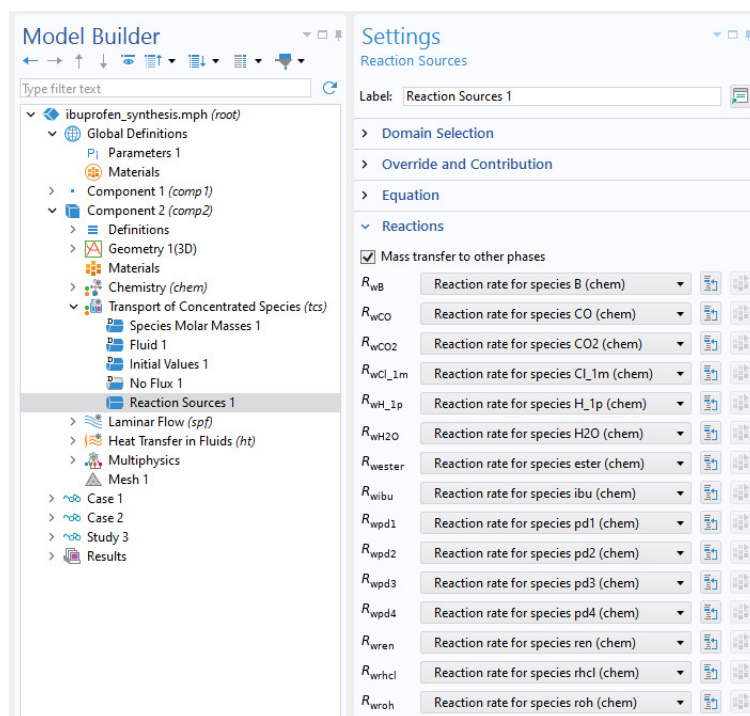


Figure 5-9: The Chemistry node generates global variables for rate variables and properties defined in the Reaction Engineering interfaces, and announces these to be used in relevant features of other space-dependent interfaces. The reaction rates within a Reaction Sources feature in a Transport of Concentrated Species interface illustrate this.

SURFACE REACTIONS

When surface species are present (that is, when the **Type** is set to **Surface species** for at least one species in the reactor), the surface reactions can be implemented in the space-dependent model in three different ways.

- When **Transport of Diluted Species in Porous Catalysts** or **Transport of Concentrated Species in Porous Catalysts** is selected, the surface reactions will be modeled using a **Surface Reaction** node under the **Porous Catalyst** feature.
- When **Transport of Diluted Species in Packed Beds** or **Transport of Concentrated Species in Packed Beds** is selected, the surface reactions will be modeled using a **Reactions** node under the subnode **Pellets** of the **Packed Bed** feature.
- When any other chemical species transport interface (except these mentioned above) is selected, the surface reactions will be modeled using a separate

Surface Reaction interface defined on the boundaries of the geometry. The surface reaction rates of species will be represented by a **Flux** feature in the created chemical species transport interface.

A feature for volumetric reactions is also added and set up, in accordance with the reaction kinetics defined in the **Reaction Engineering** interface, when clicking the **Create/Refresh** button in the **Space-Dependent Model Generation** section.

In [Figure 5-10](#), the surface reaction kinetics in a **Reacting Engineering** interface has been implemented in a **Packed Bed** feature using a **Reactions** subfeature. Note that the surface

reaction rates are defined by the **Chemistry** interface with the **Define variables for porous pellets** being checked under **Pellet Chemistry** section.

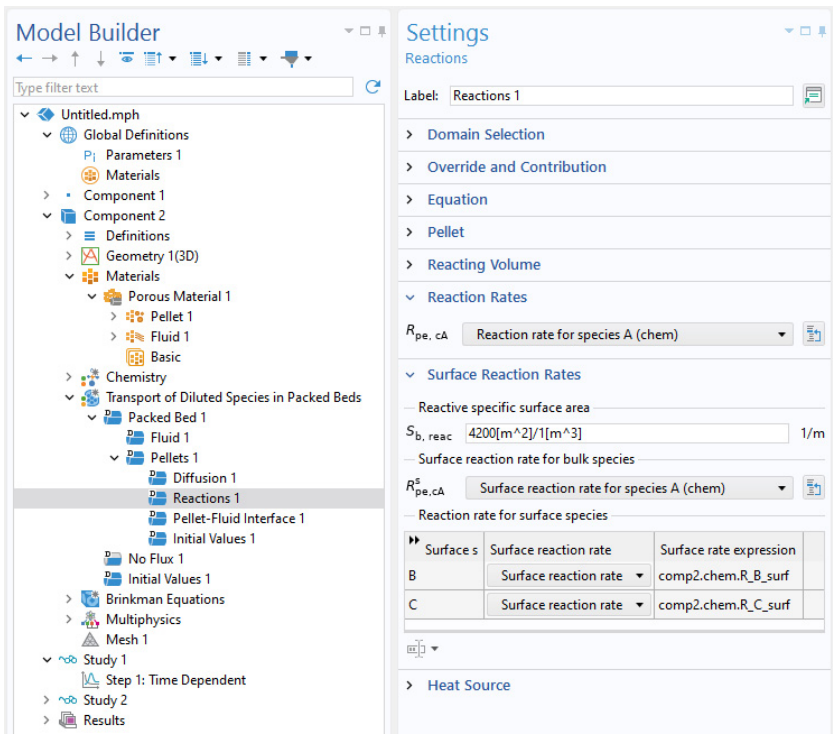


Figure 5-10: A Packed Bed feature including surface species can be automatically created, from a Reaction Engineering interface, using the Generate Space-Dependent Model feature.

-
- [The Packed Bed Feature](#)
 - [The Transport of Diluted Species Interface](#)

Chemical Species Transport

The following single physics interfaces are available with the Chemical Reaction Engineering Module:

- [The Transport of Diluted Species Interface](#)
- [The Transport of Charge Carriers Interface](#)
- [The Transport of Diluted Species in Porous Media Interface](#)

- [The Transport of Concentrated Species Interface](#)
- [The Transport of Concentrated Species in Porous Media Interface](#)
- [The Nernst–Planck Equations Interface](#)

The model generation automatically defines the dependent variables for all species. The interfaces based on transport of diluted species use default variable names according to the syntax `cspeciesname`, referring to species concentrations in mole per volume. The interfaces based on transport of concentrated species use the syntax `wspeciesname` for default variable names, referring to the species weight fraction. The initial values for the dependent species variables in the space-dependent model are based on the initial species values in the Reaction Engineering interface.

Binary diffusion coefficients can be computed and transferred to a space-dependent model. The available diffusion models for the mass balance physics interfaces sometimes require the binary diffusion coefficients of the mixture, describing all pairwise diffusion interactions between species. Under the assumption of an ideal gas the mass transfer interface for Transport of Concentrated Species can utilize the binary diffusion coefficient. The Transport of Diluted Species and Nernst-Planck Equations interfaces assume that the chemical species being transported are present in small amounts and are diluted in a solvent. The binary diffusion coefficient in these cases (in the presence of a solvent species) become the diffusion coefficient of the bulk species.

Fluid Flow

The model generation process can be selected to generate a Fluid Flow interface.

There are these separate momentum balance physics interfaces:

- [The Single-Phase Flow, Laminar Flow Interface](#)
- [The Darcy’s Law Interface](#) (in the *CFD Module User’s Guide*)
- [The Free and Porous Media Flow, Brinkman Interface](#) (in the *CFD Module User’s Guide*)

Species density (see [Equation 5-93](#), [Equation 5-94](#), and [Equation 5-95](#)) and dynamic viscosity can for some mixture options be transferred from the Reaction Engineering interface to the Fluid Flow interfaces.





NOx Reduction in a Monolithic Reactor: Application Library path
Chemical_Reaction_Engineering_Module/Tutorials/monolith_reactor

Hydrocarbon Dehalogenation in a Tortuous Microreactor: Application
Library path **Chemical_Reaction_Engineering_Module/
Reactors_with_Mass_Transfer/tortuous_reactor**

Protein Adsorption: Application Library path
**Chemical_Reaction_Engineering_Module/Mixing_and_Separation/
protein_adsorption**

Heat Transfer

In the Reaction Engineering interface, time- and space-dependent energy balance equations can also be set up. In the model generation process the physics interface generates expressions used by the Heat Transfer interface, such as the heat generated by a chemical reaction. It also generates expressions for physical transport properties.

There are two heat transfer interfaces under **Heat transfer**:

- **Heat Transfer in Fluids**
- **Heat Transfer in Porous Media**

Several expressions for the species density, heat capacity, and thermal conductivity are available and can be transferred from the Reaction Engineering interface.

The densities are available from the [Calculate Transport Properties](#) section in the interface, where the fluid mixture properties are selected. The density depends on the [Species](#) settings and is computed as follows for:

- Liquid, if assuming the liquid to be ideal and incompressible. The liquid mixture density depends on the density of i number of pure species, ρ_i , and the species weight fraction, w_i .

$$\rho = \frac{1}{\sum_i \frac{w_i}{\rho_i}} \quad (5-93)$$

The volume fraction is given by the species concentration, c_i , and the molar mass, M_i .

$$w_i = \frac{c_i M_i}{\sum_i c_i M_i} \quad (5-94)$$

- Gas mixture density depends on the concentrations and molar masses of the mixture species.

$$\rho = \sum_i c_i M_i \quad (5-95)$$

For mixtures with solvent all values are taken from the species set as solvent.

The heat capacity, c_p (SI unit: J/(mol·kg)), of the mixture is calculated by the species' molar heat capacity, C_p (SI unit: J/(mol·kg)) according to

$$c_p = \sum_i w_i \frac{C_{p,i}}{M_i} \quad (5-96)$$

where M is the molar mass (SI unit: kg/mol) and w_i the weight fraction.

Porous media type

The **Porous media type** is available when **Transport of Diluted Species in Packed Beds** or **Transport of Concentrated Species in Packed Beds** is selected for **Chemical species transport** and the **Heat Transfer in Porous Media** is selected for **Heat transfer**. There are three options the **Porous media type**:

- **Local thermal equilibrium**
- **Local thermal nonequilibrium**
- **Packed bed**



These options are the same as that for **Porous Medium** feature under **Heat Transfer in Porous Media** interface. The heat balance equation is set up inside pellets when the **Packed bed** is selected.

STUDY TYPE

Select a **Study Type**, either **Stationary** or **Time Dependent**.

The Chemistry Interface

This physics interface can be used to create reaction kinetics and optionally compute mass transport and thermodynamic properties for direct use in 1D, 2D, or 3D models. This is similar to [The Reaction Engineering Interface](#), except that it does not solve for an ideal reactor model.

The **Chemistry (chem)** interface () is found under the **Chemical Species Transport** branch () when adding a physics interface. The Chemistry interface is also created when the [Generate Space-Dependent Model](#) feature is used in the **Reaction Engineering** interface, collecting all mixture variables and properties for use in a space-dependent model.

This physics interface is a tool for generating a set of variables to be used for modeling chemical species and reactions systems. The variables are generated from species and reaction properties and can be divided in two categories:

- Rate expressions and heat sources for use in mass and heat balances.
- Material property variables (mixture density, diffusivities, viscosity, and so on) for use in space-dependent transport equations.

Many of the fields and nodes described in this section are only made available when either a [Reaction](#) or a [Species](#) (or both) subnode is added to the Model Builder. All predefined constants and expressions can be overwritten by user-defined expressions. This makes it possible to go beyond the modeling assumptions set as defaults in this physics interface.



- [Theory for the Reaction Engineering and Chemistry Interfaces](#)
- [Transport Properties](#)
- [Feature Nodes Available for the Chemistry Interface](#)

The following is a description of the features and fields available in the **Settings** window for the Chemistry interface.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern

<name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is **chem**.

MODEL INPUT

This section sets the **Temperature**, **Pressure**, and **Electrode potential** (only available with a Battery Design Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, or Fuel Cell & Electrolyzer Module license) to be used by the current interface. Use the lists to select a temperature, pressure, or electrode potential defined and announced by another interface in the model. For example, when a heat transfer interface is also included, the temperature solved for is available in the **Temperature** list.

For **Temperature** or **Pressure**, you can also select **Common model input** to use a globally available common model input. In all three cases, select **User defined** to manually define the variable in question.

MIXTURE PROPERTIES

Type

Use this setting to define specify what kind of mixture assumption is used. For **Diluted Species** the mixture is composed of low concentration solutes present in a solvent. For **Concentrated Species** a mixture where no single species is considered to be in excess is assumed.

Select **Diluted species** from the **Type** list to use the concentration variables from a Transport of Diluted Species interface in the [Species Matching](#) section. The same setting should be used for any other interface solving for molar concentrations using a diluted species assumption. Select **Concentrated species** from the **Type** list to use the mass fractions from a Transport of Concentrated Species interface.

Thermodynamics

All property parameters and property functions required by the interface can be automatically created by coupling to a system added to the **Thermodynamics** node. To do so, click the **Thermodynamics** checkbox and select an existing [Thermodynamic System](#).

The **Thermodynamics** checkbox is enabled when the [Thermodynamics](#) node, including one or more systems, is available under **Global Definitions**. Also, the Chemistry interface needs to include at least one species.

Phase

Use the **Phase** list to specify the state of aggregation of the mixture.

Density



The mixture density settings are only available when you have selected the **Calculate mixture properties** checkbox in the **Calculate Transport Properties** section.

Density always has two settings available: **Automatic** or **User defined**. The **Thermodynamics** options is available when the interface is coupled to a [Thermodynamic System](#), and all interface species has been matched to species in the system. In this case the density is defined by a function automatically added under the thermodynamic system coupled to.

The **Automatic** setting uses the following logic:

- When **Phase** is set to **Liquid**, **Automatic** assumes that the liquid is ideal and incompressible. The liquid mixture density depends on the density of i number of pure species (ρ_i) and the species weight fraction (w_i).

$$\rho = \frac{1}{\sum_i \frac{w_i}{\rho_i}}$$

The weight fraction is given by the species concentration (c_i) and the molar mass (M_i).

$$w_i = \frac{c_i M_i}{\sum_i c_i M_i}$$

- When **Phase** is set to **Gas**, **Automatic** calculates the gas mixture density (ρ) from the concentrations (c_i) and molar masses (M_i) of the mixture species, which are automatically taken from [Species](#) features.

$$\rho = \sum_i c_i M_i \quad (5-97)$$

- If the [Type](#), for one of the present species, is set to **Solvent**, and the **Mixture** is **Liquid**, the mixture density is the same as the solvent density. The species density is defined in the **General parameters** section of the corresponding Species node. When **Mixture**

is **Gas**, the mixture density is calculated from [Equation 5-97](#) only for the species set as **Solvent**.

SPECIES MATCHING

This section is used to match species solved for in space dependent physics interfaces to the species defined in Chemistry. By doing so the variables for the reaction kinetics and the mixture properties defined by Chemistry can be applied to study chemically reacting or composition dependent systems.

Species Solved For

Use this list to populate the inputs in the **Bulk species** table with dependent variables from a certain mass transfer interface. The **Species solved for** list contains all present interfaces of the **Type** selected in the **Mixture Properties** section. For example, when the **Type** is **Diluted species**, all Transport of Diluted Species interfaces or variants thereof, such as Transport of Diluted Species in Porous Media interface, are available in the list.

Bulk Species

Use the **Bulk species** table to specify the concentrations to be used as arguments in reaction kinetics variables, for example the reaction rate. Reaction kinetics variables are generated by the species features ([Species](#) and [Species Group](#)) and by the reaction features ([Reaction](#), [Reversible Reaction Group](#), and [Equilibrium Reaction Group](#)).

The bulk species concentrations are also used in the mixture properties, both for transport properties like the density and viscosity, and thermodynamic properties like the enthalpy or heat capacity.

When a mass transfer interface has been selected in the **Species solved for** list, use the **Molar concentration** column to select one of the dependent variables in the selected interface to the corresponding **Species** in Chemistry. When using a concentrated species interface (defined by the **Type** list in the [Mixture Properties](#) section), instead use the **Mass fraction** column to select a dependent variable for each species in Chemistry. For a consistent set up, the species molar mass in the Transport of Concentrated Species interface is updated to the one defined in the Chemistry interface.

The **Molar concentration** and **Mass fraction** columns also includes a **User defined** option, in which case a constant, parameter, or variable expression can be entered in the **Value** column.

Thermodynamics Coupling

When the **Thermodynamics** is enabled, the species in the Chemistry interface can be coupled to the species in the **Thermodynamic System**. This is needed to ensure that arguments for the thermodynamic functions are correctly defined. Use the lists in the **From Thermodynamics** column to match each species in the Chemistry to a species in the coupled thermodynamic system. For each thermodynamics-coupled species, the required property parameters and functions are added under the corresponding thermodynamic system. When all species are matched, the Chemistry is considered fully coupled and functions representing mixture properties, such as the density, are also added automatically under the same thermodynamic system.

Surface Species

The **Surface Species** table is available when there is at least one surface species (with “(ads)” as suffix).

Similar to the table for **Bulk Species**, the surface species can be matched (or coupled) directly to the surface species dependent variables if the Chemistry is coupled to a mass transfer interface where the surface concentration is solved. There are three cases where mass transfer interfaces solve surface species concentration (s).

- **Surface Reactions** physics interface;
- **Packed Bed** feature (with surface species transport in pellet) available in the **Transport of Diluted Species or Transport of Concentrated Species**;
- **Porous Catalyst** feature (with surface species transport in catalyst) available in the **Transport of Diluted Species or Transport of Concentrated Species**.

The last column **Value(mol/m²)** will be automatically set to **Solved for** when a surface species dependent variable is selected under the column **Surface concentration**. Otherwise for a User defined being for **Surface concentration** column, specify the concentration of surface species **Value(mol/m²)** column.

The species present in this section will not be used to define mixture properties.

Solid Species

The **Solid Species** table is available when there is at least one solid species (with “(s)” as suffix).

Specify the concentration of solid species in the table in this section.

The species present in this section will not be used to define mixture properties.

Aqueous Species

The **Aqueous Species** table is available when there is at least one aqueous species (with “(aq)” as suffix).

Specify the concentration of solid species in the table in this section.

The species present in this section will not be used to define mixture properties.

Equilibrium Reaction Rate Table

This table is only available when equilibrium reactions are present in the interface. Use the **Reaction rate** column to specify the rate for each equilibrium reaction. By doing so the postprocessing variable for the total reaction rate for each species, of form `chem.Rsum_species`, will be updated correctly. For a mass transport interface, say Transport of Diluted Species, the reaction rate needed for an equilibrium reaction is typically a dependent variable. In that case, the name of the variable can be found in the **Shape Function** section of the **Equation View** of the node.

When the Chemistry interface is created using from the **Generate Space-Dependent Model** the table is automatically set up in accordance with the added equilibrium reaction nodes.

CALCULATE TRANSPORT PROPERTIES

Select the **Calculate mixture properties** checkbox (selected as default) to calculate mixture properties that can be picked up in the space-dependent model interfaces. The properties that can be calculated are shown beneath the checkbox. There are four properties, heat capacity, ratio of specific heats, thermal conductivity and dynamic viscosity. For these properties, the **Automatic** and **User defined** are always available, the **Thermodynamics** is available when all bulk species are coupled to a **Thermodynamic System** (fully coupled). Consider also if the built-in **Automatic** expressions fit the model or if **User defined** expressions are more suitable.

The density and diffusion coefficient are always calculated.

It could be costly to calculate mixture properties by **Automatic** or **Thermodynamics** if there are a lot of species. The calculations of mixture properties are set to the **User defined** when the number of species from an imported file (chemkin file or a reaction file) exceeds the maximum number (default 200). The maximum number can be changed under the **Advanced Settings** section (activated by **Advanced Physics Options**).



Transport Properties

ACTIVITY

This section is available when the **Thermodynamics** checkbox is cleared.

Select the **Use activity** checkbox to solve for species activities instead of species concentrations, which is a common approach when nonideal fluids are modeled.

An activity coefficient other than 1 can be set for each species for the [Species](#) node in the **Species Concentration/Activity** section.



Activity

CHEMKIN IMPORT FOR SPECIES PROPERTIES

It is available when the **Thermodynamics** checkbox is cleared.

This section enables CHEMKIN[®] import to simulate complex chemical reactions in gas phase.

Two types of CHEMKIN input files can be imported here: **Thermo** and **Transport**, for thermodynamic properties and transport properties, respectively. Properties for either volumetric or surface species are supported. Click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. For **Thermo**, the imported data is directly entered in the **NASA format** fields in the [Species](#) node's **Thermodynamic Expressions** section; for **Transport**, the imported data is entered in its **Transport Expressions** section.

PELLET CHEMISTRY

Select the checkbox **Define variables for porous pellets** when the **Chemistry** interface is used to model transport and reactions in porous pellets using the **Packed Bed** feature. In this case an extra dimension, used to represent solid pellets, or particles, is present in each point of the domain. In this extra dimension both bulk and surface species concentrations are solved for. For correct pellet chemistry make sure to input the intraparticle concentrations in the **Species Matching** section. When **Define variables for porous pellets** is selected, reaction rates as well as the mixture properties defined by **Chemistry** become available in the **Packed Bed** node and its subnodes.

For more information see the [Packed Bed](#) feature in the Transport of Diluted Species interface.


Feature Nodes Available for the Chemistry Interface

The following feature nodes are available from the **Chemistry** ribbon toolbar (Windows users), **Chemistry** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Equilibrium Reaction Group
- Reaction
- Reaction Thermodynamics¹
- Reversible Reaction Group
- Species
- Species Activity
- Species Group
- Species Thermodynamics¹

¹ This is a subnode and it is only available together with a parent node.

Reaction

To add a **Reaction** node () either right-click the **Chemistry** node or in the **Chemistry** toolbar click **Reaction**.

REACTION FORMULA

Formula

Enter a chemical equation in the **Formula** field. The chemical equation should be of the format “A + B arrow C + D”. Here, A and B are reactants, C and D are product species, and arrow denotes a reaction arrow. The participating species should be written with [Valid Species Names](#). Valid reaction arrows are “<=>” for reversible reaction, “=>” for irreversible reaction, and “=” for equilibrium reaction. Species can be given trivial names, or their chemical formulas can be used as names. Examples of valid formulas are; “carbon+oxygen=>carbondioxide”, and “C(s)+O2(g)=>CO2(g)”.

Click **Apply** to make the interface examine the species taking part in the chemical equation, and automatically add the associated [Species](#) features to the Model Builder.

Balance ()

Use the **Balance** button to automatically calculate the stoichiometric coefficients such that the number of atoms of each kind are the same on both sides of the reaction. This turns, for example, the formula “H2+O2=>H2O” into “2H2+O2=>2H2O”. The balancing involves parsing all participating species for elements in the periodic table. It therefore requires that all species in the **Formula** field are written either using their chemical formula, say “H2O”, or that each species in the reaction have an enabled

Chemical Formula field in their **Species** node. For example, it is possible to balance the formula “H₂+O₂=>water” as long as there is a Species node with the name “water” already present, and an enabled **Chemical Formula**.

For automatic reaction balancing to be successful, requires that the problem is well posed. One example of a problem that is not well posed is “C+H₂=>CH₄+C₂H₆”, in which case any ratio of CH₄/C₂H₆ could be obtained. Another example is “H₂=>O₂” where not all elements are present on both sides.

Reaction Type

Select the **Reaction type** — **Reversible**, **Irreversible**, or **Equilibrium** — or edit the expression directly in the **Formula** field. In the latter case, specify the reaction type with a delimiter separating the two sides of the equation:

- <=> denotes a **Reversible** reaction
- => denotes an **Irreversible** reaction
- = denotes a reaction at chemical **Equilibrium**

Each **Reaction type** has its own set of reaction kinetics:

- If the reaction is **Reversible** or **Irreversible**, the reaction rate for reaction i contributes to the change in species i as follows:

$$R_i = \sum_j v_{ij} r_j \quad (5-98)$$

where v_{ij} is the stoichiometric coefficient.

- If it is an **Equilibrium** reaction, the equilibrium expression is equal to the equilibrium constant:

$$K_{\text{eq}} = K_{\text{eq}0}$$

REACTION RATE

This section is available when the **Reaction type** is either **Reversible** or **Irreversible**.

When **Mass action law** is selected (default), the rate expression is automatically derived from the stoichiometric coefficients in the reaction formula:

- For an **Irreversible** reaction type, the reaction rate becomes:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} \quad (5-99)$$

- For a **Reversible** reaction type, the expression instead becomes:

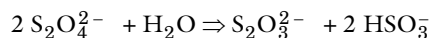
$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-\nu_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{\nu_{ij}} \quad (5-100)$$

The deduced overall reaction order is shown in text below the respective equation in the **Reaction Rate** section.

Arbitrary Rate Expression

If the reaction order differs from the stoichiometric coefficients, or if an arbitrary rate expressions is applicable, change **Reaction Rate** to **User defined**. An expression field r appears with the default expression being that from the mass action law. Below this there are fields to set the reaction order. For a reversible reaction the reverse reaction order may be specified in addition to the forward one. The unit of the rate constant k (or frequency factor A in the case of Arrhenius behavior), is derived from the reaction order, in SI units: $(\text{m}^3/\text{mol})^{\alpha-1}/\text{s}$, where α equals the order with respect to volumetric species. When surface species are present — identified by their “(ads)” suffix — the unit is instead given by $\text{m}^{3\alpha+2\beta-2}/\text{mol}^{\alpha+\beta-1}/\text{s}$, where β is the order with respect to surface species.

Consider for example the reaction:



The automatically deduced reaction order is three, however, in the case that water is the solvent, the order should probably be two. This is specified as follows:

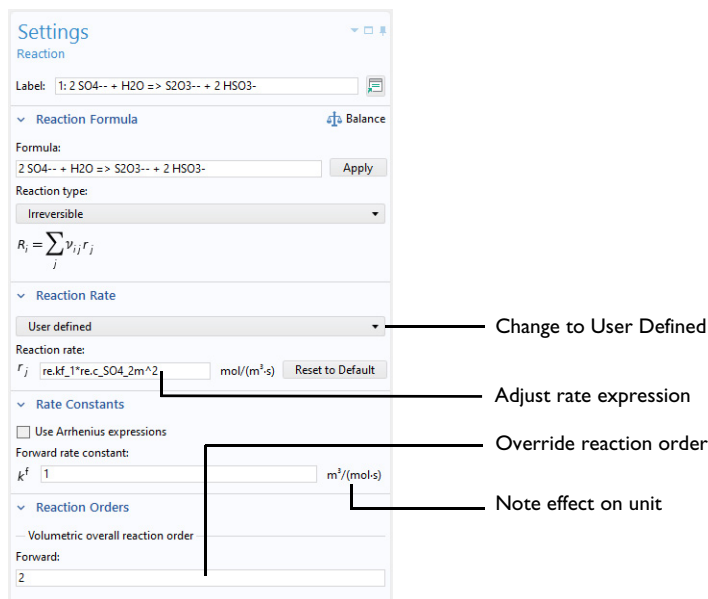


Figure 5-11: The reaction order can be manually specified for a user defined reaction rate.

RATE CONSTANTS

This section applies for **Reversible** or **Irreversible** reactions and defines the reaction rate constants used in the reaction rates.

Forward Rate Constant and Reverse Rate Constant

The **Forward rate constant** k^f is used for both **Reversible** and **Irreversible** reactions. The **Reverse rate constant** k^r is only used for **Reversible** reactions (Equation 5-99).

The SI units of the rate constants are automatically based on the order of the reaction with respect to the concentrations, as defined in the **Reaction formula**.

Specify Equilibrium Constant

The **Specify equilibrium constant** checkbox is available for **Reversible** reactions. If the checkbox is selected the rate constants are defined in a different manner with the reverse rate constant being computed from the following expression:

$$k^r = k^f / K_{\text{eq}0}$$

Thus, in this case, the forward rate constant and equilibrium constant for the reaction are needed. The **Equilibrium constant** is edited in the [Equilibrium Settings](#) section.

Use Arrhenius Expressions

When the **Use Arrhenius expressions** checkbox is selected the Arrhenius parameters are automatically used in predefined expressions for the forward and reverse rate constants k^f and k^r , respectively.

$$k^f = A^f (T/T_{\text{ref}})^{n^f} \exp(-E^f/(R_g T))$$

$$k^r = A^r (T/T_{\text{ref}})^{n^r} \exp(-E^r/(R_g T))$$

Specify the activation energy and the frequency factor in the Arrhenius expressions to account for temperature variations. The reference temperature, T_{ref} equals 1 K. The available fields are based on the **Reaction type** chosen in the [Reaction](#) node. Enter values or expressions for each of the following (reverse expressions are only available for reversible reactions):

- **Forward frequency factor** A^f and **Reverse frequency factor** A^r (unit depends on reaction order)
- **Forward temperature exponent** n^f and **Reverse temperature exponent** n^r
- **Forward activation energy** E^f and **Reverse activation energy** E^r (SI unit: J/mol)

EQUILIBRIUM SETTINGS

This section is available for equilibrium reactions, and for reversible reactions when the **Specify equilibrium constant** checkbox has been selected.

Equilibrium Expression

For an equilibrium reaction, specify the **Equilibrium expression**. When the **Equilibrium expression** is set to **Automatic** the following expression is used:

$$K_{\text{eqj}} = \frac{\prod_{i \in \text{prod}} c_i^{v_{ij}}}{\prod_{i \in \text{react}} c_i^{-v_{ij}}}$$

Select **User defined** from the **Equilibrium expression** list to instead enter a manually defined equilibrium expression.

Equilibrium Constant

Specify the **Equilibrium constant** K_{eq0} for an equilibrium reaction, or for a reversible reaction when the **Specify equilibrium constant** checkbox has been selected (in the **Rate Constants** section).

The **Equilibrium constant** can either be **User defined**, or automatically defined when set to **Automatic** or **Thermodynamics**.

Use the **Automatic** option to compute the equilibrium constant for an ideal system.

The **Thermodynamics** option is available when all reactions in the interface are equilibrium reactions, and the interface is fully coupled to a **Thermodynamic System** (see **Species Matching**). Use this setting to automatically compute the equilibrium constant for an ideal or nonideal system, dependent on the thermodynamic model applied for the coupled system.

Using **Automatic** or **Thermodynamics**, K_{eq0} is calculated from the Gibbs free energy of the reaction. For more details see **The Equilibrium Constant** and the **Automatically Defined Equilibrium Constants** section therein.

REACTION THERMODYNAMIC PROPERTIES

This section contains information about thermodynamic properties that relate to a selected reaction. Several **Automatic** definitions are available here.

Enthalpy of Reaction

The **Enthalpy of reaction** H (SI unit: J/mol) is calculated by the interface from species properties and the related stoichiometric coefficients:

$$H_j = \sum_{i \in \text{prod}} \nu_{ij} h_i - \sum_{i \in \text{react}} (-\nu_{ij}) h_i \quad (5-101)$$

Entropy of Reaction

The **Entropy of reaction** S (SI unit: J/(mol·K)) comes from a similar expression:

$$S_j = \sum_{i \in \text{prod}} \nu_{ij} s_i - \sum_{i \in \text{react}} (-\nu_{ij}) s_i \quad (5-102)$$

In **Equation 5-101** and **Equation 5-102**, h_i and s_i are the species' molar enthalpy and molar entropy, respectively.

Enter these quantities in the **Species Thermodynamic Expressions** section for the [Species](#) node either by using the predefined polynomial or by providing a custom expression or constants.

The stoichiometric coefficients, ν_{ij} , are defined as being negative for reactants and positive for products. Using [Equation 5-101](#) and [Equation 5-102](#) to equate the Gibbs free energy of reaction enables the equilibrium constant to be expressed according to [Equation 5-101](#).

Heat Source of Reaction

The **Heat source of reaction** (SI unit: W/m^3) is automatically computed from the heat of each reaction j , given by

$$Q_j = -H_j r_j$$

TURBULENT FLOW

This section is available if the following conditions are met:

- 1 Type** under **Mixture Properties** is **Concentrated species**
- 2 Reversible** or **irreversible bulk reaction**
- 3 Activity** not selected
- 4 Pellet Chemistry** not selected

When this section is activated, the **Reaction** feature can be coupled to turbulent flow in the **Transport of Concentrated Species** interface.

In a turbulent flow, there are many small turbulent eddies (known as fine structures), where actual dissipation of turbulent kinetic energy into heat and simultaneous mixing occur. The chemical reactions can take place inside these isolated regions. According to the ratio between the time scales of chemical reactions and mixing (the Damköhler number, Da), the reaction rate can be modeled in the following three ways:

- $Da \ll 1$ — the mixing process is very fast, the limiting rate step is the chemical reaction
- $Da \gg 1$ — the chemical reaction rate is very fast, the limiting rate step is the turbulent mixing rate
- Da being not far away from 1 — the reaction rate is controlled by both chemical reaction and turbulent mixing rates

The equations for the reaction rate controlled by both chemical reaction and turbulent mixing are

$$r_j^c = [\min(r_{MV,j}^{for}, r_{ED,j}^{for}) - \min(r_{MV,j}^{rev}, r_{ED,j}^{rev})]$$

$$r_{MV,j}^{for} = k^f \prod_r (c_i)^{-v_{i,r}}$$

$$r_{MV,j}^{rev} = k^r \prod_p (c_i)^{-v_{i,p}}$$

$$r_{ED,j}^{for} = \frac{\alpha}{\tau_T} \rho \min \left[\min, \beta \prod_p \frac{\omega_p}{v_p M_p} \right]$$

$$r_{ED,j}^{rev} = \frac{\alpha}{\tau_T} \rho \min \left[\min \left(\frac{\omega_p}{v_p M_p} \right), \beta \prod_r \frac{\omega_r}{v_r M_r} \right]$$

For very fast mixing process ($Da \ll 1$), the reaction rate equations are the same as that for normal reaction (without turbulence).

For very fast chemical reaction ($Da \gg 1$), the equation for reaction rate is,

$$r_j^c = r_{ED,j}^{for} - r_{ED,j}^{rev}$$

Turbulence-Reaction Model

Select a turbulent model from the combo box, for example, Eddy dissipation.

Turbulence-Reaction Model Parameters

This subsection is available when a valid turbulence model is selected in the **Turbulence-reaction model** list. There are two dimensionless parameters, α_{ED} and β_{ED} , with default values 4 and 0.5, respectively.

Turbulence Time Scale

The time scale feature input (τ_T) is available when a valid turbulence model is selected. It contains all available turbulence time scales from turbulence flow interfaces.

Assume Infinitely Fast Reaction

This checkbox is available when a valid turbulence model is selected. With the checkbox selected, the reaction rate is controlled completely by the turbulence time scale, and the **Reaction rate** list and the sections **Rate Constants** and **Reaction Orders** will be not available.

REGULARIZATION


This section is available under the same conditions as those for the **Turbulent Flow** section.

With the checkbox **Reaction rate regularization** selected, a table for **Reaction rate damping limits** will be available. For each species in the reaction, the default damping limit is 1e-6.



Using the Reaction Node

Species

When a **Reaction** is defined, a **Species** node () is automatically generated for the participating reactants and products. This feature enables you to review and enter species specific information regarding chemical kinetics, thermodynamics, and transport properties.

It is also possible to add and define an individual **Species** node: in the **Chemistry** toolbar click **Species** or right-click the **Chemistry** node and select it from the context menu.

NAME

When a **Species** node is automatically generated using the **Formula** text field for the Reaction node, the **Name** is also automatically generated.

For a **Species** node added individually, enter a **Name** in the field and click **Apply**. By entering a name consisting of elements from the periodic table, the molar mass is calculated and added in the **Chemical Formula** section. The species charge, and type, are also deduced from the species name.



Valid Species Names

TYPE

Select a species type — **Bulk species**, **Surface species**, or **Solvent**. The latter is only available when a diluted solution is assumed. That is when **Type** is set to **Diluted Species** in the **Mixture Properties** section (in the interface level).

Bulk species and **Solvent** are solved for volumetric concentrations (SI unit: mol/m³), while **Surface species** are solved for surface concentration (SI unit: mol/m²). The compositions for **Bulk species** and **Solvent** use the syntax `c_speciesname`, while **Surface species** uses `csurf_speciesname_surf`.

When **Surface species** is selected, the corresponding reaction formula introduces **(ads)** after the species notation and changes the species' name to `speciesname_surf`. Additionally, the Species node name is updated in a similar fashion.

CHEMICAL FORMULA

The **Chemical Formula** section contains the species chemical formula, **Molar mass**, *M*, and **Charge**, *z*.

If the name entered for the species consists of only elements from the periodic table, and optionally charge and phase indication, then the **Chemical Formula** field will be populated with the name entered in the **Name** section, and the molar mass and charge will be added to this section. The species molar mass is computed from the mass of occurring individual elements². The rules for writing chemical formulas are the same as those for **Species** names.



Valid Species Names

When the species name contains parts not in the periodic table, for example when a descriptive name such as **water** is used, the molar mass is set to 0.0 kg/mol and the charge to zero. In this case, the molar mass needs to be defined in order to achieve mass balanced reactions and correct definitions of mass basis properties. By entering a chemical formula consisting only of elements from the periodic table (and optionally charge and phase indication), the molar mass, and charge are derived automatically.

When needed, the **Molar mass** can be edited in the corresponding text field. Editing the **Chemical formula** and pressing apply will override the molar mass and charge fields. The **Charge** field cannot be edited as long as a chemical formula is enabled.

With an enabled **Chemical Formula** it is possible to use the trivial name of a species and balance reactions. Having added the Species **water**, **oxygen**, and **hydrogen**, and filled in **H2O**, **O**, and **H** in their respective chemical formula sections, the **Formula**

2. Values are averages of upper and lower bounds for each atom as published by CIAAW. Source: CIAAW. Atomic weights of the elements 2019. Available online at www.ciaaw.org.

oxygen+hydrogen=water is balanced into oxygen+2hydrogen=water by clicking **Balance** in the **Reaction** node.

It is possible to specify the species density ρ when the fluid **Mixture** is specified as **Liquid**. The default value is that of water at 293 K.

REACTION RATE

Change the **Automatic** default setting to **User defined** to use a species reaction rate other than the one set up in the associated **Reaction** node. For individual species, use the **User defined** option to set a reaction rate other than zero (that is, nonreactive).

Edit either the **Rate expression** (SI unit: $\text{mol}/(\text{m}^3 \cdot \text{s})$), the **Surface rate expression** (SI unit: $\text{mol}/(\text{m}^2 \cdot \text{s})$), or both. For a bulk species, both expressions appear if surface reactions are present since the reaction of the species can depend both on bulk reaction R and surface reaction R_{ads} rates. For a surface species, only the surface reaction rate R_{ads} appears.

ADDITIONAL SOURCE

The **Additional Source** section is available in order to include additional rate contribution for the species to the reaction kinetics. When the **Additional source** checkbox is selected, add an **Additional rate expression** in the text field (SI unit: mol/m^3).

CONSTANT CONCENTRATION/ACTIVITY

To account for nonideality in the fluid mixture, adjust the activity coefficient in the **Activity coefficient** input field. This input field is only shown if activity instead of concentration has been chosen in the interface, that is, the **Use activity** checkbox is selected on the Chemistry interface **Settings** window

Click to select the **Keep concentration/activity constant** checkbox if the species concentration or activity should be treated as constant.

TRANSPORT EXPRESSIONS

Here the required parameters to compute various transport properties can be edited. To show this section the **Calculate mixture properties** checkbox needs to be selected under the **Calculate Transport Properties** section.

- For a gas mixture, there are maximum five properties to consider: σ , the characteristic length (unit: Å) of the Lennard–Jones/Stockmayer potential; ϵ/k_{B} , the energy minimum (SI unit: K) of the Lennard–Jones/Stockmayer potential; μ_{D} , the dipole moment (SI unit: Debye); k_i , the thermal conductivity of the gas (SI unit:

W/(m·K)); and Diffusivity of the species (SI unit: m²/s). The latter two can be set as **Automatic**, when theoretical Transport Parameters expressions are available.

- For mixtures of gas with solvent, all properties above except the thermal conductivity is shown. This is instead calculated under the **Calculate mixture properties** section in the Settings window for the Chemistry interface.
- For a liquid mixture, there is only the parameter k_i , the thermal conductivity (SI unit: W/(m·K)) to edit.
- For mixtures of liquid with solvent, the thermal conductivity is shown only for the species set as **Solvent**.

THERMODYNAMIC EXPRESSIONS

The parameters utilized for calculation of thermodynamic mixture and reaction properties are set in this section.

The **Thermodynamic Expressions** are by default computed using data input in the **NASA format**. In this case, enter the following to compute the species' heat capacity, C_p (SI unit: J/(mol·K)), the molar enthalpy, h (SI unit: J/mol), and the molar entropy, s (SI unit: J/(mol·K)):

- **Lower temperature limit** T_{lo}
- **Middle temperature limit** T_{mid}
- **Upper temperature limit** T_{hi}
- **Polynomial coefficients** $a_{low,k}$ and $a_{hi,k}$


Any coefficients for the thermodynamic polynomials entered into the $a_{low,k}$ fields apply to the temperatures in the range T_{lo} to T_{mid} ; coefficients entered into the $a_{hi,k}$ fields apply to temperatures in the range T_{mid} to T_{hi} range. The coefficients can also be imported in the **CHEMKIN Import for Species Properties** section in the Chemistry node.

Choose the **User defined** alternative to specify C_p , h , and s directly.



Using the Species Node

Reversible Reaction Group







The **Reversible Reaction Group** node () allows input of a large number of reversible reactions in the same table. All reactions are treated in the same way. More than one Reversible Reaction Group can be added to a component. The feature is typically used when importing CHEMKIN kinetics files.

Add the node from the **Chemistry** toolbar or right-click **Chemistry** and add it from the context menu.

For the case when reaction kinetics data are entered manually into the **Reaction table** and temperature dependent reaction kinetics apply, right-click to add a [Reaction Thermodynamics](#) subnode or select it from the **Chemistry** toolbar, **Attributes** menu. In it, the Enthalpy of Reaction (J/mol) for each reaction can be specified.

REACTION TABLE

The reversible reactions in the **Reaction table** are numbered and contain reactants, products, and kinetic parameters describing the reaction. Use the buttons under the **Reaction table** to add and sort the reaction details.

- In general, use the **Move Up** (), **Move Down** (), and **Delete** () buttons and the fields under tables to edit the table contents. Or right-click a table cell and select **Move Up**, **Move Down**, or **Delete**.
- The **Add** button () adds default reactant, A, and product, B, with a default. Click the corresponding field to edit the reactant, product, or parameters. After editing the [Species Group](#) node is also updated. It is created together with the reaction group.
- You can save the parameters to a text file to reuse in other models. Click the **Save to File** button () and enter a **File name** in the **Save to File** dialog, including the extension .txt. Click **Save** to store the parameters in a text file or in a Microsoft Excel Workbook spreadsheet if the license includes LiveLink™ for Excel®. The information is saved in space-separated columns in the same order as displayed on screen. When saving to Excel, an **Excel Save** dialog appears where you can specify the sheet and range and whether to overwrite existing data or include a header.
- You can import or load data in files from a spreadsheet program, for example, with the **Load from File** button () and the **Load from File** dialog that appears. Data must be separated by spaces or tabs. If there is already data in the table, imported parameters are added after the last row. Move or edit rows as needed. If the license includes LiveLink™ for Excel® you can also load parameters from a Microsoft Excel Workbook spreadsheet. Then an **Excel Load** dialog appears where you can specify the

sheet and range and whether to overwrite existing data. It is also possible to import from a spreadsheet containing a separate column for units.

CREATE REACTION AND SPECIES

Enter a reaction number in the **Moving reaction (with the number) from table** text field and click **Create Reaction** to remove the reaction from the **Reaction table** to the model tree. This introduces a reaction node named after the reaction number and species names and simultaneously creates corresponding species nodes. This action is powerful, since it enables all the editing possibilities available for [Reaction](#) and [Species](#) nodes.


CHEMKIN IMPORT FOR KINETICS

Click to select the **Import CHEMKIN data** checkbox to import a CHEMKIN **Kinetics input file**. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**.



CHEMKIN Data and NASA Polynomials

Equilibrium Reaction Group







The **Equilibrium Reaction Group** node () allows for input of a large number of equilibrium reactions in the same table. This node functions in the same way as the [Reversible Reaction Group](#) for reversible reactions.

Add the node from the **Chemistry** toolbar or right-click **Chemistry** and add it from the context menu.


For the case when reaction kinetics data are entered manually into the **Reaction table** and temperature dependent reaction kinetics apply, right-click to add a [Reaction Thermodynamics](#) subnode or select it from the **Chemistry** toolbar, **Attributes** menu. In it, the Enthalpy of Reaction (J/mol) for each reaction can be specified.

REACTION TABLE

The equilibrium reactions in the table are numbered and contain reactants, products, and kinetic parameters describing the reaction. Use the buttons under the **Reaction table** to add and sort the reaction details.

- In general, use the **Move Up** (), **Move Down** (), and **Delete** () buttons and the fields under tables to edit the table contents. Or right-click a table cell and select **Move Up**, **Move Down**, or **Delete**.
- The **Add** button () adds default reactant, A, and product, B, with a default. Click the corresponding field to edit the reactant, product, or parameters. After editing the **Species Group** node is also updated. It is created together with the reaction group.
- You can save the parameters to a text file to reuse in other models. Click the **Save to File** button () and enter a **File name** in the **Save to File** dialog, including the extension .txt. Click **Save** to store the parameters in a text file or in a Microsoft Excel Workbook spreadsheet if the license includes LiveLink™ for Excel®. The information is saved in space-separated columns in the same order as displayed on screen. When saving to Excel, an **Excel Save** dialog appears where you can specify the sheet and range and whether to overwrite existing data or include a header.
- You can import or load data in files from a spreadsheet program, for example, with the **Load from File** button () and the **Load from File** dialog that appears. Data must be separated by spaces or tabs. If there is already data in the table, imported parameters are added after the last row. Move or edit rows as needed. If the license includes LiveLink™ for Excel® you can also load parameters from a Microsoft Excel Workbook spreadsheet. Then an **Excel Load** dialog appears where you can specify the sheet and range and whether to overwrite existing data. It is also possible to import from a spreadsheet containing a separate column for units.

Species Group

The **Species Group** node () contains information on a molecular level about the volumetric species and the surface species present in the model. The **Property for Volumetric Species** or **Property for Surface Species** tables typically collect parameters from when importing CHEMKIN transport files.

This node is automatically added when either the **Reversible Reaction Group** or the **Equilibrium Reaction Group** is used.

For the case of temperature dependent reaction kinetics, a [Species Thermodynamics](#) subnode is automatically created in which the thermodynamic properties of the species can be specified.

CHEMKIN

This section allows import of CHEMKIN transport files. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. Note that this section is only shown when transport properties are computed (**Calculate mixture properties** checkbox under the **Calculate Transport Properties** is selected).



- [CHEMKIN Data and NASA Polynomials](#)
-

Reaction Thermodynamics

The **Reaction Thermodynamics** subnode (), the Enthalpy of Reaction (J/mol) of each reaction can be specified. This node overrides all the automatically calculated reaction enthalpies as defined in the [Species Thermodynamics](#) subnode.

Add the **Reaction Thermodynamics** node from the **Chemistry** toolbar, **Attributes** menu. Alternatively, right-click a [Reversible Reaction Group](#) or [Equilibrium Reaction Group](#) to add the **Reaction Thermodynamics** subnode.

Species Activity

The **Species Activity** node () creates variables for the activities of all the species/surface species present in the Species Group parent feature. Edit the **Activity coefficient** field in the **Species Activity** or **Surface Species Activity** tables by clicking in these.

Species Activity is a subnode to the [Species Group](#) node. It is automatically generated when nonideality in the fluid mixture is accounted for; when the **Use activity** checkbox is selected in the **Activity** section.

Species Thermodynamics

The **Species Thermodynamics** node () creates variables for the enthalpies, entropies, and heat capacities for all the species/surface species present in the [Species Group](#)

parent feature. The purpose is to compute thermodynamic mixture properties and the heat of reactions.

This node is a subnode to the [Species Group](#) node.

THERMODYNAMIC PROPERTIES OF SPECIES

Select a **Type selection** for the thermodynamic properties. The **NASA format** alternative requires the setting of several polynomial constants and is typically used together with CHEMKIN import. The **User defined** alternative only requires input of Species molar enthalpy (J/mol) and Species molar capacity (J/(mol·K)).


CHEMKIN IMPORT FOR THERMODYNAMIC DATA

This section allows import of thermodynamic CHEMKIN transport files. To import the data directly into the table columns, click **Browse** to locate the CHEMKIN file to be imported, then click **Import**. Note that this can only be done for the **NASA format** option.



- [CHEMKIN Data and NASA Polynomials](#)
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Radio Frequency Interfaces

This chapter discusses the physics interfaces found under the **Radio Frequency** branch ()

In this chapter:

- [The Electromagnetic Waves, Transient Interface](#)
- [The Transmission Line, Transient Interface](#)

The Electromagnetic Waves, Transient Interface

The **Electromagnetic Waves, Transient (temw)** interface () , found under the **Radio Frequency** branch () when adding a physics interface, is used to solve a time-domain wave equation for the magnetic vector potential. The sources can be in the form of point dipoles, line currents, or incident fields on boundaries or domains. It is primarily used to model electromagnetic wave propagation in different media and structures when a time-domain solution is required — for example, for nonsinusoidal waveforms or for nonlinear media. Typical applications involve the propagation of electromagnetic pulses.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Wave Equation**, **Electric**, **Perfect Electric Conductor**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Electromagnetic Waves, Transient** to select physics features from the context menu.

Except where indicated, most of the settings are the same as for [The Electromagnetic Waves, Frequency Domain Interface](#).

Physics-Controlled Mesh

The physics-controlled mesh is controlled from the **Settings** window for the **Mesh** node (if the **Sequence type** is **Physics-controlled mesh**). In the table in the **Physics-Controlled Mesh** section, find the physics interface in the **Contributor** column and select or clear the checkbox in the **Use** column on the same row for enabling (the default) or disabling contributions from the physics interface to the physics-controlled mesh.

When the **Use** checkbox for the physics interface is selected, this invokes a parameter for the maximum mesh element size in free space. The physics-controlled mesh automatically scales the maximum mesh element size as the wavelength changes in different dielectric and magnetic regions. If the model is configured by any periodic conditions, identical meshes are generated on each pair of periodic boundaries. Perfectly matched layers are built with a structured mesh, specifically, a swept mesh in 3D and a mapped mesh in 2D.

When the **Use** checkbox is selected for the physics interface, in the section for the physics interface below the table, choose one of the four options for the **Maximum mesh**

element size control parameter — **User defined** (the default), **Frequency**, or **Wavelength**. For the option **User defined**, enter a suitable **Maximum element size in free space**. For example, $1/5$ of the vacuum wavelength or smaller. When **Frequency** is selected, enter the highest frequency intended to be used during the simulation. The maximum mesh element size in free space is $1/8$ in 2D and $1/5$ in 3D of the vacuum wavelength for the entered frequency. For the **Wavelength** option, enter the smallest vacuum wavelength intended to be used during the simulation. The maximum mesh element size in free space is $1/8$ in 2D and $1/5$ in 3D of the entered wavelength.

The maximum mesh element sizes discussed above are used with quadratic shape functions. When linear shape functions are used, $1/2$ of the maximum mesh element size for quadratic shape functions are used. Similarly, when cubic shape functions are used, the maximum mesh element size is 2.25 times the maximum mesh element size for quadratic shape functions.

Furthermore, for Lumped Port features, the maximum mesh element size can be slightly finer than what is discussed above.

The maximum mesh element size in dielectric media is equal to the maximum mesh element size in vacuum divided by the square root of the product of the relative permittivity and permeability.

When **Refine conductive edges** is selected, the exterior edges of conductive boundaries, configured by perfect electric conductors, transition boundary, or layered transition boundary conditions, are meshed with a user-specified size. Adjust **Angular tolerance** (SI unit: rad) to include not only edges on flat surfaces but also curved surfaces. Choose **Size type** — **Relative** or **User defined**. For the option **Relative**, the mesh size on the selected edges is defined relative to the default maximum mesh size. On the other hand, when the option **User defined** is selected, the mesh size is set by user-defined value in the **Size** input field (SI unit: m).

When **Add far-field boundary layers** is selected, the far-field calculation boundaries adjacent to the selection of scattering boundary conditions or perfectly matched layers create a boundary layer mesh with a thickness of $1/40$ to the default maximum mesh size.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to

different physics interfaces, the **name** string must be unique. Only letters, numbers, and underscores (**_**) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is **temw**.

COMPONENTS

This section is available for 2D and 2D axisymmetric components.

Select the **Electric field components solved for**. Select:


- **Three-component vector** (the default) to solve using a full three-component vector for the electric field **E**.
- **Out-of-plane vector** to solve for the electric field vector component perpendicular to the modeling plane, assuming that there is no electric field in the plane.
- **In-plane vector** to solve for the electric field vector components in the modeling plane assuming that there is no electric field perpendicular to the plane.

DEPENDENT VARIABLES

The dependent variable (field variable) is for the **Magnetic vector potential A**. The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

Select the shape order for the **Magnetic vector potential** dependent variable — **Linear**, **Quadratic** (the default), **Cubic**, **Quartic**, **Quintic**, **Sextic**, or **Septic**. For more information about the **Discretization** section, see [Settings for the Discretization Sections](#) in the *COMSOL Multiphysics Reference Manual*.

	<ul style="list-style-type: none">• Domain, Boundary, Edge, Point, and Pair Nodes for the Electromagnetic Waves, Transient Interface• Theory for the Electromagnetic Waves Interfaces
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Domain, Boundary, Edge, Point, and Pair Nodes for the Electromagnetic Waves, Transient Interface

The [Electromagnetic Waves, Transient Interface](#) shares most of its nodes with [The Electromagnetic Waves, Frequency Domain Interface](#).

The domain, boundary, edge, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

These nodes are unique for this physics interface and described in this section:

- [Wave Equation, Electric](#)
- [Initial Values](#)
- [Drude–Lorentz Polarization](#)
- [Far-Field Domain](#)
- [Far-Field Calculation](#)

BOUNDARY CONDITIONS

With no surface currents present the boundary conditions

$$\mathbf{n}_2 \times (\mathbf{E}_1 - \mathbf{E}_2) = \mathbf{0}$$

$$\mathbf{n}_2 \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{0}$$

need to be fulfilled. Depending on the field being solved for, it is necessary to analyze these conditions differently. When solving for **A**, the first condition can be formulated in the following way.

$$\mathbf{n}_2 \times (\mathbf{E}_1 - \mathbf{E}_2) = \mathbf{n}_2 \times \left(\frac{\partial \mathbf{A}_2}{\partial t} - \frac{\partial \mathbf{A}_1}{\partial t} \right) = \frac{\partial}{\partial t} (\mathbf{n}_2 \times (\mathbf{A}_2 - \mathbf{A}_1))$$

The tangential component of the magnetic vector potential is always continuous and thus the first condition is fulfilled. The second condition is equivalent to the natural boundary condition.

$$-\mathbf{n} \times (\mu_r^{-1} \nabla \times \mathbf{A}_1 - \mu_r^{-1} \nabla \times \mathbf{A}_2) = -\mathbf{n} \times \mu_r^{-1} (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{0}$$

and is therefore also fulfilled.

These nodes and subnodes are available and described for the Electromagnetic Waves, Frequency Domain interface (listed in alphabetical order):

- [Archie’s Law](#)
- [Lumped Port](#)
- [Magnetic Field](#)
- [Perfect Electric Conductor](#)
- [Perfect Magnetic Conductor](#)
- [Periodic Condition](#)
- [Effective Medium](#)
- [Scattering Boundary Condition](#)
- [Surface Current Density](#)

EDGE, POINT, AND PAIR

These edge, point, and pair nodes are available and described for the Electromagnetic Waves, Frequency Domain interface (listed in alphabetical order):

- [Edge Current](#)
- [Electric Point Dipole](#) (2D and 3D components)
- [Line Current \(Out-of-Plane\)](#) (2D and 2D axisymmetric components)
- [Magnetic Point Dipole](#) (2D and 3D components)
- [Perfect Electric Conductor](#)
- [Perfect Magnetic Conductor](#)
- [Surface Current Density](#)



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at $r = 0$) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.



In the *COMSOL Multiphysics Reference Manual* see [Table 2-4](#) for links to common sections and [Table 2-5](#) to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Wave Equation, Electric

The **Wave Equation, Electric** node is the main node for the Electromagnetic Waves, Transient interface. The governing equation can be written in the form

$$\mu_0 \sigma \frac{\partial \mathbf{A}}{\partial t} + \mu_0 \epsilon_0 \frac{\partial}{\partial t} \left(\epsilon_r \frac{\partial \mathbf{A}}{\partial t} \right) + \nabla \times (\mu_r^{-1} \nabla \times \mathbf{A}) = 0$$

for transient problems with the constitutive relations $\mathbf{B} = \mu_0 \mu_r \mathbf{H}$ and $\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E}$. Other constitutive relations can also be handled for transient problems. The **Divergence Constraint** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

ELECTRIC DISPLACEMENT FIELD

Select an **Electric displacement field model** — **Relative permittivity** (the default), **Refractive index**, **Polarization**, **Remanent electric displacement**, or **Drude-Lorentz dispersion model**.

Relative Permittivity

When **Relative permittivity** is selected, the default **Relative permittivity** ϵ_r (dimensionless) takes values **From material**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** and enter values or expressions in the field or matrix. If **Effective medium** is selected, the **Effective medium** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

Refractive Index

When **Refractive index** is selected, the default **Refractive index** n (dimensionless) takes the value **From material**. To specify the refractive index and assume a relative permeability of unity and zero conductivity, for one or both of the options, select **User defined** then choose **Isotropic**, **Diagonal**, **Symmetric**, or **Full**. Enter values or expressions in the field or matrix.



Notice that only the real part of the refractive index is used for the transient formulation.

Polarization

For **Polarization** enter coordinates for the **Polarization** \mathbf{P} (SI unit: C/m²).

Remanent Electric Displacement

For **Remanent electric displacement** enter coordinates for the **Remanent electric displacement** \mathbf{D}_r (SI unit: C/m²). Then select **User defined** or **From Material** as above for the **Relative permittivity** ϵ_r .

Drude–Lorentz Dispersion Model

For **Drude–Lorentz dispersion model** select **User defined** or **From material** for the **Relative permittivity, high-frequency** ϵ_∞ and enter a value for the **Plasma frequency** ω_p (SI unit: rad/s).

When **Drude–Lorentz dispersion model** is selected, the **Drude–Lorentz Polarization** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. Each **Drude–Lorentz Polarization** subnode adds another polarization term \mathbf{P}_n to the electric displacement field \mathbf{D} , defined by

$$\mathbf{D} = \epsilon_0 \epsilon_\infty \mathbf{E} + \sum_{n=1}^N \mathbf{P}_n,$$

where the polarization is the solution to the ordinary differential equation

$$\left(\frac{\partial^2}{\partial t^2} + \Gamma_n \frac{\partial}{\partial t} + \omega_n^2 \right) \mathbf{P}_n = \epsilon_0 f_n \omega_p^2 \mathbf{E}.$$

For more information, see the [Drude–Lorentz Polarization](#) feature.

MAGNETIC FIELD

This section is available if **Relative permittivity**, **Polarization**, or **Remanent electric displacement** are chosen as the **Electric displacement field model**.

Select the **Constitutive relation** — **Relative permeability** (the default), **Remanent flux density**, or **Magnetization**.

Relative Permeability

For **Relative permeability** the relative permeability μ_r uses values **From material**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the magnetic field, and then enter values or expressions in the field or matrix. If **Effective medium** is selected, the **Effective medium** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

Remanent Flux Density

For **Remanent flux density** the relative permeability μ_r uses values **From material**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the magnetic field, and then enter values or expressions in the field or matrix. Then enter coordinates for the **Remanent flux density** \mathbf{B}_r (SI unit: T).

Magnetization

For **Magnetization** enter coordinates for **M** (SI unit: A/m).

B-H Curve

Select **B-H curve** **|B|** (SI unit: T) to use a curve that relates magnetic field **H** and the magnetic flux density **B** as $|\mathbf{B}| = f(|\mathbf{H}|) \mathbf{H} / |\mathbf{H}|$. The **Magnetic field norm** setting can take the values **From material** or **User defined**.

Material properties from [Nonlinear Magnetic Material Library](#) can be used for **B-H curve** that are generally provided as interpolation functions for the magnetization curve without hysteresis effects.



Nonlinear simulations with the **B-H curve** magnetic field constitutive relation may require customized time-stepping settings in the **Time-Dependent Solver** for stability. The **BDF** method, with constant maximum step constraint, user-defined maximum step, and low maximum BDF order such as 2, would provide better convergence.

CONDUCTION CURRENT

This section is available if **Relative permittivity**, **Polarization**, **Remanent electric displacement**, or **Drude-Lorentz dispersion model** are chosen as the **Electric displacement field model**.

By default, the **Electric conductivity** σ (SI unit: S/m) uses values **From material**.

- For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the current and enter values or expressions in the field or matrix.
- For **Linearized resistivity** the default values for the **Reference temperature** T_{ref} (SI unit: K), **Resistivity temperature coefficient** α (SI unit: 1/K), and **Reference resistivity** ρ_0 (SI unit: Ωm) use values **From material**. For **User defined** enter other values or expressions for any of these variables.
- If **Effective medium** is selected, the **Effective medium** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.
- If **Archie's Law** is selected, the **Archie's Law** subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

Initial Values

The **Initial Values** node adds an initial value for the magnetic vector potential and its time derivative that serves as initial conditions for the transient simulation.

INITIAL VALUES

Enter values or expressions for the initial values of the components of the magnetic vector potential \mathbf{A} (SI unit: Wb/m) and its time derivative $\partial\mathbf{A}/\partial t$ (SI unit: V/m). The default values are 0 Wb/m and 0 V/m, respectively.

Drude–Lorentz Polarization

This subfeature is available only when **Drude-Lorentz Dispersion Model** is selected as the **Electric displacement field model** in the [Wave Equation, Electric](#) feature node. Then the subnodes are made available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Each **Drude-Lorentz Polarization** subnode adds another polarization term \mathbf{P}_n to the electric displacement field \mathbf{D} , defined by

$$\mathbf{D} = \epsilon_0 \epsilon_\infty \mathbf{E} + \sum_{n=1}^N \mathbf{P}_n,$$

where the polarization is the solution to the ordinary differential equation

$$\left(\frac{\partial^2}{\partial t^2} + \Gamma_n \frac{\partial}{\partial t} + \omega_n^2 \right) \mathbf{P}_n = \epsilon_0 f_n \omega_p^2 \mathbf{E}.$$


Here Γ_n is a damping coefficient, ω_n is a resonance frequency, f_n is an oscillator strength, and ω_p is the plasma frequency.

Enter values or expressions for the **Oscillator strength** f_n (SI unit: 1), the **Resonance frequency** ω_n (SI unit: rad/s), and the **Damping in time** coefficient Γ_n (SI unit: rad/s).

INITIAL VALUES

Enter values or expressions for the initial values of the components of the Drude–Lorentz polarization \mathbf{P}_n (SI unit: C/m²) and its time derivative $\partial\mathbf{P}_n/\partial t$ (SI unit: A/m²).



DISCRETIZATION

To display this section, click the **Show More Options** button () and select **Discretization** from the **Show More Options** dialog. Select the element order from the list box for the Drude–Lorentz polarization \mathbf{P}_n .



Time-Domain Modeling of Dispersive Drude–Lorentz Media:
Application Library path **RF_Module/Tutorials/drude_lorentz_media**

The Transmission Line, Transient Interface

The **Transmission Line, Transient (tlt)** interface () found under the **Radio Frequency** branch () when adding a physics interface, is used to study propagation of waves in time domain along one-dimensional transmission lines. The physics interface solves the time-domain transmission line equation for the electric potential.

The physics interface is used when solving for electromagnetic wave propagation along one-dimensional transmission lines and is available in 1D, 2D, and 3D. The physics interface has the Time Dependent study step available. The Time Dependent study is used for a time-dependent source driven simulations for a single frequency.

When the physics interface is added, three default nodes are also added to the **Model Builder** — **Transmission Line Equation**, **Open Circuit**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Transmission Line, Transient** to select physics features from the context menu.

Physics-Controlled Mesh

The physics-controlled mesh is controlled from the **Settings** window for the **Mesh** node (if the **Sequence type** is **Physics-controlled mesh**). In the table in the **Physics-Controlled Mesh** section, find the physics interface in the **Contributor** column and select or clear the checkbox in the **Use** column on the same row for enabling (the default) or disabling contributions from the physics interface to the physics-controlled mesh.

When the **Use** checkbox for the physics interface is selected, this invokes a parameter for the maximum mesh element size in the transmission line. The physics-controlled mesh automatically scales the maximum mesh element size as the wavelength changes in different transmission lines. If the model consists of multiple transmission lines, identical number of domain mesh elements are generated in each of them.

When the **Use** checkbox is selected for the physics interface, in the section for the physics interface below the table, choose one of the three options for the **Maximum mesh element size control parameter** — **User defined** (the default), **Frequency**, or **Wavelength**. When **User defined** is selected, enter a suitable **Maximum element size in free space**. For example, 1/5 of the vacuum wavelength or smaller, and it scales the value to the transmission line wavelength. When **Frequency** is selected, enter the highest

frequency intended to be used during the simulation. The maximum mesh element size is $1/60$ of the transmission line wavelength for the entered frequency. For the **Wavelength** option, enter the smallest vacuum wavelength intended to be used during the simulation. The maximum mesh element size is $1/60$ of the transmission line wavelength.



In the *COMSOL Multiphysics Reference Manual* see the [Physics-Controlled Mesh](#) section for more information about how to define the physics-controlled mesh.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern `<name>.<variable_name>`. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (`_`) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is `t1t`.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Electric potential V** (SI unit: V). The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION




Select the shape order for the **Electric potential** dependent variable — **Linear**, **Quadratic** (the default), or **Cubic**. For more information about the **Discretization** section, see [Settings for the Discretization Sections](#) in the *COMSOL Multiphysics Reference Manual*.



- [Domain, Boundary, Edge, Point, and Pair Nodes for the Transmission Line, Transient Equation Interface](#)
- [Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide](#)
- [Visualization and Selection Tools](#) in the *COMSOL Multiphysics Reference Manual*

Domain, Boundary, Edge, Point, and Pair Nodes for the Transmission Line, Transient Equation Interface

The [Transmission Line, Transient Interface](#) has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

	In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the Attributes menu.
	Select Edges for 3D models, Boundaries for 2D models, and Domains for 1D models. Points are available for all space dimensions (3D, 2D, and 1D). For all space dimensions, select Points for the boundary condition.
<div><div><ul style="list-style-type: none">• Transmission Line Equation• Initial Values• Absorbing Boundary• Incoming Wave</div><div><ul style="list-style-type: none">• Open Circuit• Terminating Impedance• Short Circuit• Lumped Port</div></div>	
	Theory for the Transmission Line, Transient Boundary Conditions in the <i>RF Module User's Guide</i>

Transmission Line Equation

The **Transmission Line Equation** node is the main feature of the Transmission Line, Transient interface. It defines the 1D wave equation for the electric potential in time domain. The wave equation is written as

$$LC \frac{\partial^2 V}{\partial t^2} + (RC + LG) \frac{\partial V}{\partial t} - \nabla^2 V + RGV = 0$$

where R , L , G , and C are the distributed resistance, inductance, conductance, and capacitance, respectively, and $\frac{\partial}{\partial t}$ is the partial derivative with respect to time.

TRANSMISSION LINE EQUATION

Enter the values for the following:

- **Distributed resistance R** (SI unit: m·kg/(s³·A²)). The default is 0 m·kg/(s³·A²).
- **Distributed inductance L** (SI unit: H/m). The default is 2.5e-6 H/m.
- **Distributed conductance G** (SI unit: S/m). The default is 0 S/m.
- **Distributed capacitance C** (SI unit: F/m). The default is 1e-9 F/m.

Initial Values

The **Initial Values** node adds an initial value for the electric potential and the first time derivative of the electric potential that can serve as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter values or expressions for the initial values of the **Electric potential V** (SI unit: V) and **Electric potential, first time derivative $\frac{\partial V}{\partial t}$** (SI unit: V/s).

Absorbing Boundary

The **Absorbing Boundary** condition is stated as

$$\frac{1}{L} \frac{\partial V}{\partial x} + \sqrt{\frac{C}{L}} \frac{\partial V}{\partial t} + \frac{1}{2L} \frac{RC + LG}{\sqrt{LC}} V = 0$$

where **n** is the normal pointing out of the domain. The *absorbing boundary* condition prescribes that propagating waves are absorbed at the boundary and, thus, that there is no reflection at the boundary. The Absorbing Boundary condition is only available on external boundaries.



Theory for the Transmission Line, Transient Boundary Conditions in the
RF Module User’s Guide

Incoming Wave

The **Incoming Wave** boundary condition

$$\sqrt{\frac{C}{L}} \frac{\partial V}{\partial t} + \frac{\mathbf{n} \cdot \nabla V}{L} + \frac{1}{2L} \frac{RC + LG}{\sqrt{LC}} V - 2 \sqrt{\frac{C}{L}} \frac{\partial V_{\text{in}}}{\partial t} - \frac{1}{L} \frac{RC + LG}{\sqrt{LC}} V_{\text{in}} = 0$$

lets a time-dependent wave V_{in} enter the domain. The outward-pointing normal \mathbf{n} is defined in the section describing the [Absorbing Boundary](#) node. The Incoming Wave boundary condition is only available on external boundaries.

VOLTAGE

Select a voltage source **Type** for the input **Electric potential** V_{in} (SI unit: V)—**Sinusoidal** (the default) or **User defined**.

- If a **Sinusoidal** type is selected under **Voltage**, enter the **Frequency** f_0 (SI unit: Hz) and **Amplitude** V_0 (SI unit: V). The default **Frequency** is 1 GHz and the default **Amplitude** is 1 V.
- If an **User defined** type is selected under **Voltage**, enter the expression for the input **Electric potential** V_{in} (SI unit: V). The default expression is $\sin(2\pi f_0 t)$ V where f_0 is 1 GHz.



[Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide](#)

Open Circuit

The **Open Circuit** boundary condition is a special case of the [Terminating Impedance](#) boundary condition, assuming an infinite impedance, and, thus, zero current at the boundary. The condition is thus

$$\mathbf{n} \cdot \nabla V = 0$$

The Open Circuit boundary condition is only available on external boundaries.



[Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide](#)

Terminating Impedance


The **Terminating Impedance** boundary condition

$$\frac{1}{Z_L} \frac{\partial V}{\partial t} + \frac{\mathbf{n} \cdot \nabla V}{L} + \frac{R}{L Z_L} V = 0$$

specifies the terminating impedance to be Z_L . The Terminating Impedance boundary condition is only available on external boundaries.

IMPEDANCE


Enter the value or expression for the **Impedance** Z_L (SI unit: Ω). The default is 50 Ω .


	Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide
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Short Circuit

The **Short Circuit** node is a special case of the [Terminating Impedance](#) boundary condition, assuming that impedance is zero and, thus, the electric potential is zero. The constraint at this boundary is, thus, $V = 0$.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button () and select **Advanced Physics Options** in the **Show More Options** dialog.

	Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide
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Lumped Port

Use the **Lumped Port** node to apply a voltage or current excitation to a domain.

PORT PROPERTIES

Enter a unique **Port Name**. It is recommended to use a numeric name.

Select a **Type of Port** — **Cable** (the default) or **Current**.


If a **Cable** is selected as the port type, select the **Wave excitation at this port** — **On** (the default) or **Off**. Select **On** to apply a voltage excitation to a domain.

If **On** is selected as the **Wave excitation at this port**, select the **Voltage source type** for the input **Electric potential** V_{in} (SI unit: V) — **Sinusoidal** (the default) or **User defined**.

- If a **Sinusoidal** type is selected as the **Voltage source type**, enter the **Frequency** f_0 (SI unit: Hz) and **Amplitude** V_0 (SI unit: V). The default **Frequency** is 1 GHz and the default **Amplitude** is 1 V.
- If an **User defined** type is selected under **Voltage**, enter the expression for the input **Electric potential** V_{in} (SI unit: V). The default expression is $\sin(2\pi f_0 t)$ V where f_0 is 1 GHz

SETTINGS

- If a **Cable** port type is selected under **Port Properties**, enter the **Characteristic impedance** Z_{ref} (SI unit: Ω). The default is 50 Ω .
- If a **Current** terminal type is selected under **Port Properties**, enter the expression of a **Terminal current** I_{in} (SI unit: A). The default expression is $\sin(2\pi f_0 t)$ A where f_0 is 1 GHz.

	<ul style="list-style-type: none">• S-Parameters and Ports• Lumped Ports with Voltage Input• Theory for the Transmission Line, Transient Boundary Conditions in the RF Module User's Guide
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