Plasma Module

User’s Guide
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Contents

Chapter 1: Introduction

About the Plasma Module ........................................ 12
Why Plasma is Used in Modeling ................................. 12
How the Plasma Module Helps Improve Your Modeling ...... 13
Plasma Module Nomenclature ...................................... 14
The Plasma Module Physics Guide ............................... 16
Where Do I Access the Documentation and Model Libraries? 19

Overview of the User's Guide .................................. 23

Chapter 2: Data Required for Plasma Modeling

Data Requirements ............................................... 26
Electron Impact Reactions ....................................... 26
Reaction .................................................................. 27
Surface Reaction .................................................... 27
Species .................................................................. 28

Importing Collision Cross-Section Data ....................... 30
Cross-Section Data File Format .................................. 30
The File Format ...................................................... 31
Reference for the Plasma Module Cross-Section Data Requirements .... 33

Chapter 3: The AC/DC Branch

The Electrostatics Interface ....................................... 36
Domain, Boundary, Edge, Point, and Pair Nodes for the
    Electrostatics Interface ....................................... 38
Charge Conservation ............................................... 40
Initial Values ....................................................... 41
Space Charge Density .......................... 42
Zero Charge .................................. 42
Ground ........................................ 43
Electric Potential .............................. 44
Surface Charge Density ...................... 46
External Surface Charge Accumulation .......... 46
Electric Displacement Field .................... 47
Periodic Condition ............................ 48
Thin Low Permittivity Gap ..................... 49
Surface Charge Accumulation ................... 49
Dielectric Shielding ............................ 50
Terminal ....................................... 51
Floating Potential .............................. 52
Distributed Capacitance ....................... 54
Line Charge .................................... 54
Line Charge (on Axis) .......................... 55
Line Charge (Out-of-Plane) ..................... 56
Point Charge ................................... 56
Point Charge (on Axis) .......................... 57
Change Cross-Section .......................... 58
Change Thickness (Out-of-Plane) ............... 59
Electrostatic Point Dipole ...................... 59

The Electrical Circuit Interface .................. 61
Ground Node .................................... 62
Resistor ........................................ 63
Capacitor ...................................... 63
Inductor ........................................ 63
Voltage Source .................................. 64
Current Source .................................. 65
Voltage-Controlled Voltage Source .............. 66
Voltage-Controlled Current Source .............. 66
Current-Controlled Voltage Source .............. 67
Current-Controlled Current Source .............. 67
Subcircuit Definition ............................ 68
Subcircuit Instance ............................. 68
NPN BJT ........................................ 69
n-Channel MOSFET ............................. 69
Chapter 4: The Fluid Flow Branch

The Single-Phase Flow, Laminar Flow Interface 98
The Laminar Flow Interface 98
Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow 101
<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid Properties</td>
<td>102</td>
</tr>
<tr>
<td>Volume Force</td>
<td>103</td>
</tr>
<tr>
<td>Initial Values</td>
<td>104</td>
</tr>
<tr>
<td>Wall</td>
<td>104</td>
</tr>
<tr>
<td>Inlet</td>
<td>107</td>
</tr>
<tr>
<td>Outlet</td>
<td>111</td>
</tr>
<tr>
<td>Symmetry</td>
<td>113</td>
</tr>
<tr>
<td>Open Boundary</td>
<td>114</td>
</tr>
<tr>
<td>Boundary Stress</td>
<td>115</td>
</tr>
<tr>
<td>Vacuum Pump</td>
<td>116</td>
</tr>
<tr>
<td>Periodic Flow Condition</td>
<td>118</td>
</tr>
<tr>
<td>Flow Continuity</td>
<td>119</td>
</tr>
<tr>
<td>Point Mass Source</td>
<td>119</td>
</tr>
<tr>
<td>Line Mass Source</td>
<td>120</td>
</tr>
<tr>
<td>Pressure Point Constraint</td>
<td>121</td>
</tr>
<tr>
<td>Theory for the Single-Phase Flow Laminar Interface</td>
<td>123</td>
</tr>
<tr>
<td>General Single-Phase Flow Theory</td>
<td>124</td>
</tr>
<tr>
<td>Compressible Flow</td>
<td>126</td>
</tr>
<tr>
<td>The Mach Number Limit</td>
<td>126</td>
</tr>
<tr>
<td>Incompressible Flow</td>
<td>127</td>
</tr>
<tr>
<td>The Reynolds Number</td>
<td>127</td>
</tr>
<tr>
<td>The Boussinesq Approximation</td>
<td>128</td>
</tr>
<tr>
<td>Theory for the Wall Boundary Condition</td>
<td>129</td>
</tr>
<tr>
<td>Prescribing Inlet and Outlet Conditions</td>
<td>132</td>
</tr>
<tr>
<td>Laminar Inflow</td>
<td>133</td>
</tr>
<tr>
<td>Laminar Outflow</td>
<td>134</td>
</tr>
<tr>
<td>Mass Flow</td>
<td>135</td>
</tr>
<tr>
<td>No Viscous Stress</td>
<td>136</td>
</tr>
<tr>
<td>Pressure, No Viscous Stress Boundary Condition</td>
<td>137</td>
</tr>
<tr>
<td>Normal Stress Boundary Condition</td>
<td>138</td>
</tr>
<tr>
<td>Pressure Boundary Condition</td>
<td>138</td>
</tr>
<tr>
<td>Vacuum Pump Boundary Condition</td>
<td>139</td>
</tr>
<tr>
<td>Mass Sources for Fluid Flow</td>
<td>141</td>
</tr>
<tr>
<td>Numerical Stability—Stabilization Techniques for Fluid Flow</td>
<td>143</td>
</tr>
<tr>
<td>Solvers for Laminar Flow</td>
<td>145</td>
</tr>
<tr>
<td>Pseudo Time Stepping for Laminar Flow Models</td>
<td>147</td>
</tr>
<tr>
<td>Discontinuous Galerkin Formulation</td>
<td>149</td>
</tr>
</tbody>
</table>
Chapter 5: The Boltzmann Equation, Two-Term Approximation Interface

The Boltzmann Equation, Two-Term Approximation Interface 154
Domain, Boundary, and Pair Nodes for the Boltzmann Equation, Two-Term Approximation Interface 157
Boltzmann Model 158
Initial Values 159
Collision 160
Boundary Settings 161
Zero Energy Flux 162
Zero Probability 162

Theory for the Boltzmann Equation, Two-Term Approximation Interface 163
The Electron Energy Distribution Function 163
Boltzmann Equation, Two-Term Approximation 164
References for the Boltzmann Equation, Two-Term Approximation Interface 170

Chapter 6: The Drift Diffusion Interface

The Drift Diffusion Interface 172
Domain, Boundary, and Pair Nodes for the Drift Diffusion Interface 174
Drift Diffusion Model 175
Initial Values 178
Electron Production Rate 178
General Power Deposition 179
Velocity 179
Inductive Power Deposition 179
Microwave Power Deposition 180
## Chapter 7: The Heavy Species Transport Interface

<table>
<thead>
<tr>
<th>The Heavy Species Transport Interface</th>
<th>194</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain, Boundary, and Pair Nodes for the Heavy Species Transport Interface</td>
<td>198</td>
</tr>
<tr>
<td>Cross Section Import</td>
<td>199</td>
</tr>
<tr>
<td>Diffusion and Migration</td>
<td>199</td>
</tr>
<tr>
<td>Electron Impact Reaction</td>
<td>200</td>
</tr>
<tr>
<td>Reaction</td>
<td>204</td>
</tr>
<tr>
<td>Species</td>
<td>205</td>
</tr>
<tr>
<td>Surface Reaction</td>
<td>209</td>
</tr>
<tr>
<td>Surface Species</td>
<td>211</td>
</tr>
<tr>
<td>Flux</td>
<td>212</td>
</tr>
<tr>
<td>Inlet</td>
<td>212</td>
</tr>
<tr>
<td>Outflow</td>
<td>213</td>
</tr>
<tr>
<td>Symmetry</td>
<td>214</td>
</tr>
</tbody>
</table>

| Theory for the Heavy Species Transport Interface                           | 215 |
| About the Transport Equations                                              | 215 |
Chapter 8: The Plasma Reactor Interfaces

The Capacitively Coupled Plasma Interface

Domain, Boundary, Edge, Point, and Pair Physics for the Capacitively Coupled Plasma Interface

Plasma Model

Initial Values

Continuity on Interior Boundary

The DC Discharge Interface

The Inductively Coupled Plasma Interface

Domain, Boundary, Point, and Pair Physics for the Inductively Coupled Plasma Interface

Plasma Model

Collisionless Heating

Initial Values

Gauge Fixing for A-field

The Microwave Plasma Interface

Domain, Boundary, Edge, Point, and Pair Physics for the Microwave
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma Interface</td>
<td>258</td>
</tr>
<tr>
<td>Initial Values</td>
<td>259</td>
</tr>
<tr>
<td><strong>Plasma Reactors Theory</strong></td>
<td>261</td>
</tr>
<tr>
<td><strong>Theory for the Capacitively Coupled Plasma Interface</strong></td>
<td>264</td>
</tr>
<tr>
<td><strong>Theory for the DC Discharge Interface</strong></td>
<td>266</td>
</tr>
<tr>
<td>Introduction to DC Discharge Theory</td>
<td>266</td>
</tr>
<tr>
<td>DC Discharge Interface Boundary Conditions</td>
<td>267</td>
</tr>
<tr>
<td>Tips for Modeling DC Discharges</td>
<td>268</td>
</tr>
<tr>
<td><strong>Theory for the Inductively Coupled and Microwave Plasma Interfaces</strong></td>
<td>269</td>
</tr>
<tr>
<td>Introduction to Inductively Coupled Plasmas</td>
<td>269</td>
</tr>
<tr>
<td>Domain Equations for the Inductively Coupled Plasma Interface</td>
<td>271</td>
</tr>
<tr>
<td>Wave Heated Discharge Theory</td>
<td>272</td>
</tr>
<tr>
<td>Domain Equations for the Microwave Plasma Interface</td>
<td>273</td>
</tr>
<tr>
<td>Plasma Conductivity in the Presence of a Static Magnetic Field</td>
<td>273</td>
</tr>
</tbody>
</table>
Introduction

This guide describes the Plasma Module, an optional add-on package that extends the COMSOL Multiphysics® modeling environment with customized physics interfaces and functionality optimized for the analysis of non-equilibrium discharges.

This chapter introduces you to the capabilities of this module. 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.

• About the Plasma Module
• Overview of the User’s Guide
About the Plasma Module

A number of physics interfaces for plasma modeling form the backbone of the module. These physics interfaces are based on a pair of drift-diffusion equations for the electron density and mean electron energy, an extended form of the Maxwell-Stefan equations for the nonelectron species (referred to as “heavy species”), and an electrostatics model to compute the plasma potential. There is also a physics interface that solves a two-term approximation to the Boltzmann equation.

In general, the coupling between the individual physics interfaces is rather complicated. To facilitate the modeling process there are four predefined multiphysics interfaces for the most common types of plasmas. The complicated coupling between the individual physics interfaces is automatically handled by the software when using these multiphysics interfaces. The following topics are described further in this chapter:

In this section:
- Why Plasma is Used in Modeling
- How the Plasma Module Helps Improve Your Modeling
- Plasma Module Nomenclature
- The Plasma Module Physics Guide
- Where Do I Access the Documentation and Model Libraries?

Why Plasma is Used in Modeling

Low-temperature plasmas represent the amalgamation of fluid mechanics, reaction engineering, physical kinetics, heat transfer, mass transfer, and electromagnetics. The Plasma Module is a specialized tool for modeling non-equilibrium discharges which occur in a wide range of engineering disciplines. There are specialized physics interfaces for the most common types of plasma reactors including inductively coupled plasmas (ICP), DC discharges, wave heated discharges (microwave plasmas), and capacitively coupled plasmas (CCP).
Modeling the interaction between the plasma and an external circuit is an important part of understanding the overall characteristics of a discharge. This module has tools to add circuit elements directly to a 1D, 2D, or 3D model, or import an existing SPICE netlist into the model. The plasma chemistry is specified by loading in sets of collision cross sections from a file or by adding reactions and species to the Model Builder. The complicated coupling between the different physics that constitute a plasma is automatically handled by the included multiphysics interfaces.

**How the Plasma Module Helps Improve Your Modeling**

The Plasma Module is based on a series of scientific publications on numerical modeling of non-equilibrium discharges. These papers are referenced throughout the documentation. The physics interfaces can model low temperature, non-equilibrium discharges such as:

- Inductively coupled plasmas (ICP)
- Capacitively coupled plasmas (CCP)
- Microwave plasmas
- Light sources
- Electrical breakdown
- Space thrusters
- DC discharges
- Chemical vapor deposition (CVD)
- Plasma-enhanced chemical vapor deposition (PECVD)
- Dielectric barrier discharges (DBD)
- Electron cyclotron resonance (ECR)
- Reactive gas generators

The complexity of plasma modeling lies in the fact that it combines elements of reaction engineering, statistical physics, fluid mechanics, physical kinetics, heat transfer, mass transfer, and electromagnetics. The net result is a true multiphysics problem involving complicated coupling between the different physics. The module is designed to simplify the process of setting up a self-consistent model of a low-temperature plasma.

The physics interfaces include all the necessary tools to model plasma discharges, beginning with a Boltzmann Equation, Two-Term Approximation solver that computes the electron transport properties and source coefficients from a set of
electron impact collision cross sections. This interface makes it possible to determine many of the interesting characteristics of a discharge by providing input properties such as the electric field and the electron impact reactions that make up the plasma chemistry, without solving a space-dependent problem.

For space-dependent models, the reactions and species which make up the plasma chemistry are conveniently managed in the Model Builder. When the fluid velocity and gas temperature are of interest, there are physics interfaces available for laminar flow and heat transfer. There are several options available when coupling the charged species transport to the electromagnetic fields. Poisson’s equation for the electrostatic potential is always solved. Modeling inductively coupled plasmas where induction currents are responsible for sustaining the plasma requires the AC/DC Module. For wave-heated discharges (microwave plasmas), the RF Module is required.

Plasma Module Nomenclature

The Plasma Module has numerous variables and expressions used throughout the documentation and in COMSOL Multiphysics. Table 1-1 lists the variable, its description and its SI unit.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>Gas density</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>$M_k$</td>
<td>Molecular weight, species $k$</td>
<td>kg/mol</td>
</tr>
<tr>
<td>$M_n$</td>
<td>Mean molar mass</td>
<td>kg/mol</td>
</tr>
<tr>
<td>$w_k$</td>
<td>Mass fraction, species $k$</td>
<td>1</td>
</tr>
<tr>
<td>$W_k$</td>
<td>Log of the mass fraction of species $k$</td>
<td>-</td>
</tr>
<tr>
<td>$x_k$</td>
<td>Mole fraction, species $k$</td>
<td>1</td>
</tr>
<tr>
<td>$V_k$</td>
<td>Multicomponent diffusion velocity, species $k$</td>
<td>m/s</td>
</tr>
<tr>
<td>$j_k$</td>
<td>Diffusive flux vector, species $k$</td>
<td>kg/(m$^2$·s)</td>
</tr>
<tr>
<td>$D_{kj}$</td>
<td>Binary diffusion coefficient</td>
<td>m$^2$/s</td>
</tr>
<tr>
<td>$D_{k,n}$</td>
<td>Mixture averaged diffusion coefficient</td>
<td>m$^2$/s</td>
</tr>
<tr>
<td>$D_k^T$</td>
<td>Multicomponent thermal diffusion coefficient</td>
<td>kg/(m·s)</td>
</tr>
<tr>
<td>$D_{k,f}$</td>
<td>Diffusion coefficient for species $k$</td>
<td>m$^2$/s</td>
</tr>
<tr>
<td>$Z_k$</td>
<td>Charge, species $k$</td>
<td>1</td>
</tr>
</tbody>
</table>
ABOUT THE PLASMA MODULE

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
<th>SI UNIT</th>
</tr>
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<tbody>
<tr>
<td>$\mu_{k,m}$</td>
<td>Mixture averaged mobility, species $k$</td>
<td>m$^2$/(V·s)</td>
</tr>
<tr>
<td>$V$</td>
<td>Electric potential</td>
<td>V</td>
</tr>
<tr>
<td>$E$</td>
<td>Electric field</td>
<td>V/m</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant</td>
<td>J/(mol·K)</td>
</tr>
<tr>
<td>$c_k$</td>
<td>Molar concentration, species $k$</td>
<td>mol/m$^3$</td>
</tr>
<tr>
<td>$r_j$</td>
<td>Reaction rate, reaction $j$</td>
<td>mol/(m$^3$·s)</td>
</tr>
<tr>
<td>$k_j$</td>
<td>Rate coefficient, reaction $j$</td>
<td>m$^3$/(mol·s)</td>
</tr>
<tr>
<td>$R_k$</td>
<td>Rate expression, species $k$</td>
<td>kg/(m$^3$·s)</td>
</tr>
<tr>
<td>$n_k$</td>
<td>Number density, species $k$</td>
<td>1/m$^3$</td>
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<tr>
<td>$\nu_{k,j}$</td>
<td>Stoichiometric matrix, forward component</td>
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</tr>
<tr>
<td>$\nu_{k,j}''$</td>
<td>Stoichiometric matrix, reverse component</td>
<td>1</td>
</tr>
<tr>
<td>$\nu_{kJ}$</td>
<td>Total stoichiometric matrix</td>
<td>1</td>
</tr>
<tr>
<td>$q$</td>
<td>Unit charge</td>
<td>C</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann constant</td>
<td>J/K</td>
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<tr>
<td>$R_{surf,k}$</td>
<td>Surface rate expression for species $k$</td>
<td>mol/(m$^2$·s)</td>
</tr>
<tr>
<td>$\gamma_j$</td>
<td>Sticking coefficient, reaction $j$</td>
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</tr>
<tr>
<td>$\rho_k$</td>
<td>Mass concentration, species $k$</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$u$</td>
<td>Mass averaged fluid velocity vector</td>
<td>m/s</td>
</tr>
<tr>
<td>$F$</td>
<td>Faraday’s constant</td>
<td>sA/mol</td>
</tr>
<tr>
<td>$N_A$</td>
<td>Avogadro constant</td>
<td>1/mol</td>
</tr>
<tr>
<td>$v_T$</td>
<td>Thermal drift velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>$u$</td>
<td>Mass averaged velocity field, x/r-component</td>
<td>m/s</td>
</tr>
<tr>
<td>$v$</td>
<td>Mass averaged velocity field, y/z-component</td>
<td>m/s</td>
</tr>
<tr>
<td>$w$</td>
<td>Mass averaged velocity field, z-component</td>
<td>m/s</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Surface charge density</td>
<td>C</td>
</tr>
<tr>
<td>$\Gamma_e$</td>
<td>Electron flux</td>
<td>1/(m$^2$·s)</td>
</tr>
<tr>
<td>$q_j$</td>
<td>Surface reaction rate, reaction $j$</td>
<td>mol/(m$^2$·s)</td>
</tr>
<tr>
<td>$A_j$</td>
<td>Frequency factor, reaction $j$</td>
<td>m$^3$/(mol·s)</td>
</tr>
<tr>
<td>$\beta_j$</td>
<td>Temperature exponent, reaction $j$</td>
<td>1</td>
</tr>
<tr>
<td>$E_j$</td>
<td>Activation energy, reaction $j$</td>
<td>J/mol</td>
</tr>
<tr>
<td>$f(w)$</td>
<td>Electron energy distribution function (EEDF)</td>
<td>eV$^{-3/2}$</td>
</tr>
</tbody>
</table>
The Plasma Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the Plasma Module are listed in the table. The functionality of the COMSOL Multiphysics base package is given in the *COMSOL Multiphysics Reference Manual*.

### TABLE 1-1: NOMENCLATURE USED THROUGHOUT THE PLASMA MODULE DOCUMENTATION.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
<th>SI UNIT</th>
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<tbody>
<tr>
<td>$\varepsilon$</td>
<td>Electron energy</td>
<td>eV</td>
</tr>
<tr>
<td>$\bar{\varepsilon}$, $\overline{\varphi}$</td>
<td>Mean electron energy</td>
<td>eV</td>
</tr>
<tr>
<td>$\mu_e$</td>
<td>Electron mobility</td>
<td>$m^2/(V \cdot s)$</td>
</tr>
<tr>
<td>$N_n$</td>
<td>Neutral number density</td>
<td>$1/m^3$</td>
</tr>
<tr>
<td>$\mu_r N_n$</td>
<td>Reduced electron mobility</td>
<td>$s^2 \cdot A/(m^2 \cdot kg)$</td>
</tr>
</tbody>
</table>

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 Guide*.

<table>
<thead>
<tr>
<th>INTERFACE</th>
<th>ICON</th>
<th>TAG</th>
<th>SPACE DIMENSION</th>
<th>AVAILABLE PRESET STUDY TYPE</th>
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<tbody>
<tr>
<td><strong>AC/DC</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electrical Circuit</td>
<td></td>
<td>cir</td>
<td>Not space dependent</td>
<td>stationary; frequency domain; time dependent</td>
</tr>
<tr>
<td>Electrostatics$^1$</td>
<td></td>
<td>es</td>
<td>all dimensions</td>
<td>stationary; time dependent</td>
</tr>
</tbody>
</table>

| **Fluid Flow**     |      |     |                 |                                               |
| **Single-Phase Flow** |      |     |                 |                                               |
| Laminar Flow$^1$   |      | spf | 3D, 2D, 2D axisymmetric | stationary; time dependent                   |
There are several general options available for the physics interfaces and for individual nodes. This section is a short overview of these options, and includes links to additional information.

To display additional options for the physics interfaces and other parts of the model tree, click the **Show** button ( ) on the **Model Builder** and then select the applicable option.

**SHOW MORE PHYSICS OPTIONS**

The links to the features described in the *COMSOL Multiphysics Reference Manual* (or any external guide) do not work in the PDF, only from the online help in COMSOL Multiphysics.

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<table>
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</tr>
<tr>
<td>Drift Diffusion</td>
<td>dd</td>
<td>all dimensions</td>
<td>time dependent</td>
<td></td>
</tr>
<tr>
<td>Heavy Species Transport</td>
<td>hs</td>
<td>all dimensions</td>
<td>time dependent</td>
<td></td>
</tr>
<tr>
<td>Boltzmann Equation, Two-Term Approximation</td>
<td>be</td>
<td>1D</td>
<td>frequency domain; mean energies; reduced electric fields</td>
<td></td>
</tr>
<tr>
<td>Capacitively Coupled Plasma</td>
<td>ccp</td>
<td>all dimensions</td>
<td>time dependent</td>
<td></td>
</tr>
<tr>
<td>DC Discharge</td>
<td>dc</td>
<td>all dimensions</td>
<td>time dependent</td>
<td></td>
</tr>
<tr>
<td>Inductively Coupled Plasma(^2)</td>
<td>icp</td>
<td>3D, 2D, 2D axisymmetric</td>
<td>frequency-transient</td>
<td></td>
</tr>
<tr>
<td>Microwave Plasma(^3)</td>
<td>mwp</td>
<td>3D, 2D, 2D axisymmetric</td>
<td>frequency-transient</td>
<td></td>
</tr>
</tbody>
</table>

\(^1\) This physics interface is included with the core COMSOL package but has added functionality for this module.

\(^2\) 3D is available with the addition of the AC/DC Module.

\(^3\) Requires the addition of the RF Module.
After clicking the Show button ( ), additional sections are displayed on the settings window when a node is clicked and additional nodes are made available.

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 additional sections that can be displayed include Equation, Advanced Settings, Discretization, Consistent Stabilization, and Inconsistent Stabilization.

You can also click the Expand Sections button ( ) in the Model Builder to always show some sections or click the Show button ( ) and select Reset to Default to reset to display only the Equation and Override and Contribution sections.

For most nodes, both the Equation and Override and Contribution sections are always available. Click the Show button ( ) and then select Equation View to display the Equation View node under all nodes in the Model Builder.

Availability of each node, and whether it is described for a particular node, is based on the individual selected. For example, the Discretization, Advanced Settings, Consistent Stabilization, and Inconsistent Stabilization sections are often described individually throughout the documentation as there are unique settings.

<table>
<thead>
<tr>
<th>SECTION</th>
<th>CROSS REFERENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Show More Options and Expand Sections</td>
<td>Advanced Physics Sections</td>
</tr>
<tr>
<td></td>
<td>The Model Builder</td>
</tr>
<tr>
<td>Discretization</td>
<td>Show Discretization</td>
</tr>
<tr>
<td></td>
<td>Discretization (Node)</td>
</tr>
<tr>
<td>Discretization—Splitting of complex variables</td>
<td>Compile Equations</td>
</tr>
<tr>
<td>Consistent and Inconsistent Stabilization</td>
<td>Stabilization</td>
</tr>
<tr>
<td></td>
<td>Numerical Stabilization</td>
</tr>
<tr>
<td>Constraint Settings</td>
<td>Weak Constraints and Constraint Settings</td>
</tr>
<tr>
<td>Override and Contribution</td>
<td>Physics Exclusive and Contributing Node Types</td>
</tr>
</tbody>
</table>
OTHER COMMON SETTINGS

At the main level, some of the common settings found (in addition to the Show options) are the Interface Identifier, Domain Selection, Boundary Selection, Edge Selection, Point Selection, and Dependent Variables.

At the node level, some of the common settings found (in addition to the Show options) are Domain Selection, Boundary Selection, Edge Selection, Point Selection, Material Type, Coordinate System Selection, and Model Inputs. Other sections are common based on application area and are not included here.

<table>
<thead>
<tr>
<th>SECTION</th>
<th>CROSS REFERENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coordinate System Selection</td>
<td>Coordinate Systems</td>
</tr>
<tr>
<td>Domain, Boundary, Edge, and Point Selection (geometric entity selection)</td>
<td>About Geometric Entities</td>
</tr>
<tr>
<td></td>
<td>About Selecting Geometric Entities</td>
</tr>
<tr>
<td></td>
<td>The Geometry Entity Selection Sections</td>
</tr>
<tr>
<td>Equation</td>
<td>Physics Nodes—Equation Section</td>
</tr>
<tr>
<td>Interface Identifier</td>
<td>Predefined and Built-In Variables</td>
</tr>
<tr>
<td></td>
<td>Variable Naming Convention and Namespace</td>
</tr>
<tr>
<td></td>
<td>Viewing Node Names, Identifiers, Types, and Tags</td>
</tr>
<tr>
<td>Material Type</td>
<td>Materials</td>
</tr>
<tr>
<td>Model Inputs</td>
<td>About Materials and Material Properties</td>
</tr>
<tr>
<td></td>
<td>Selecting Physics</td>
</tr>
<tr>
<td></td>
<td>Model Inputs and Multiphysics Couplings</td>
</tr>
<tr>
<td>Pair Selection</td>
<td>Identity and Contact Pairs</td>
</tr>
<tr>
<td></td>
<td>Continuity on Interior Boundaries</td>
</tr>
</tbody>
</table>

Where Do I Access the Documentation and Model Libraries?

A number of Internet resources provide more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or
context-based) help, and the Model 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 a model or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to other modules (as long as you have a license), model examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The COMSOL Multiphysics Reference Manual describes all core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions about how to use COMSOL and how to access the electronic Documentation and Help content.

Opening Topic-Based Help

The Help window is useful as it is connected to many of the features on the GUI. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then displays information about that feature (or click a node in the Model Builder followed by the Help button (7)). This is called topic-based (or context) help.

To open the Help window:
• In the Model Builder, click a node or window and then press F1.
• On any toolbar (for example, Home or Geometry), hover the mouse over a button (for example, Browse Materials or Build All) and then press F1.
• From the File menu, click Help (7).
• In the upper-right part of the COMSOL Desktop, click the (7) button.

To open the Help window:
• In the Model Builder, click a node or window and then press F1.
• On the main toolbar, click the Help (7) button.
• From the main menu, select Help>Help.
Opening the Documentation Window

To open the Documentation window:
- Press Ctrl+F1.
- From the File menu select Help>Documentation.

THE MODEL LIBRARIES WINDOW

Each model includes documentation that has the theoretical background and step-by-step instructions to create the model. The models are available in COMSOL as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual models as a template for your own modeling and applications. In most models, SI units are used to describe the relevant properties, parameters, and dimensions in most examples, but other unit systems are available.

Once the Model Libraries window is opened, you can search by model name or browse under a module folder name. Click to highlight any model of interest and a summary of the model and its properties is displayed, including options to open the model or a PDF document.

Opening the Model Libraries Window

To open the Model Libraries window ( ):

- From the Home ribbon, click ( ) Model Libraries.
- From the File menu select Model Libraries.

To include the latest versions of model examples, from the File>Help menu, select ( ) Update COMSOL Model Library.

- On the main toolbar, click the Model Libraries ( ) button.
- From the main menu, select Windows>Model Libraries.

To include the latest versions of model examples, from the Help menu select ( ) Update COMSOL Model Library.

CONTACTING COMSOL BY EMAIL

For general product information, contact COMSOL at info@comsol.com.

To receive technical support from COMSOL for the COMSOL products, please contact your local COMSOL representative or send your questions to support@comsol.com. An automatic notification and case number is sent to you by email.

COMSOL WEBSITES

<table>
<thead>
<tr>
<th>Service</th>
<th>Website</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMSOL website</td>
<td><a href="http://www.comsol.com">www.comsol.com</a></td>
</tr>
<tr>
<td>Contact COMSOL</td>
<td><a href="http://www.comsol.com/contact">www.comsol.com/contact</a></td>
</tr>
<tr>
<td>Support Center</td>
<td><a href="http://www.comsol.com/support">www.comsol.com/support</a></td>
</tr>
<tr>
<td>Product Download</td>
<td><a href="http://www.comsol.com/support/download">www.comsol.com/support/download</a></td>
</tr>
<tr>
<td>Product Updates</td>
<td><a href="http://www.comsol.com/support/updates">www.comsol.com/support/updates</a></td>
</tr>
<tr>
<td>COMSOL Community</td>
<td><a href="http://www.comsol.com/community">www.comsol.com/community</a></td>
</tr>
<tr>
<td>Events</td>
<td><a href="http://www.comsol.com/events">www.comsol.com/events</a></td>
</tr>
<tr>
<td>COMSOL Video Gallery</td>
<td><a href="http://www.comsol.com/video">www.comsol.com/video</a></td>
</tr>
<tr>
<td>Support Knowledge Base</td>
<td><a href="http://www.comsol.com/support/knowledgebase">www.comsol.com/support/knowledgebase</a></td>
</tr>
</tbody>
</table>
Overview of the User’s Guide

The Plasma 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 Model 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 of Terms, and Index. See also Plasma Module Nomenclature in this chapter.

DATA REQUIREMENTS FOR PLASMA MODELING

The Data Required for Plasma Modeling chapter describes the Data Requirements to model low-temperature plasmas. It gives an overview of the data you need to assemble before attempting to model a plasma. It also includes the section Importing Collision Cross-Section Data.

AC/DC PHYSICS INTERFACES

The AC/DC Branch chapter describes the two interfaces available with this module under the AC/DC branch when adding a physics interface. Use The Electrostatics Interface to compute the electrostatic field in the plasma caused by separation of space charge between the electrons and ions. The Plasma Module enhances the interface included with the basic COMSOL license. Use The Electrical Circuit Interface to add an external electrical circuit to the plasma model.

FLUID FLOW PHYSICS INTERFACES

The Fluid Flow Branch describes the Laminar Flow interface, which has a few additional features available for this module.

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION INTERFACE

The Boltzmann Equation, Two-Term Approximation Interface chapter describes the physics interface, which computes the electron energy distribution function (EEDF) from a set of collision cross sections for some mean discharge conditions. Additionally,
electron source coefficients and transport properties can be computed. 1D models only. The underlying theory is included at the end of the chapter.

**DRIFT DIFFUSION INTERFACE**

The Drift Diffusion Interface chapter describes the underlying electron transport theory for the Drift Diffusion interface and details the available features. Use the Drift Diffusion interface to compute the electron density and mean electron energy for any type of plasma. A wide range of boundary conditions are available to handle secondary emission, thermionic emission, and wall losses. The underlying theory is included at the end of the chapter.

**THE HEAVY SPECIES INTERFACE**

The Heavy Species Transport Interface chapter describes the interface, which is a mass balance interface for all non-electron species. This includes charged, neutral, and electronically excited species. The interface also allows you to add electron impact reactions, chemical reactions, surface reactions, and species via the Model Builder. The underlying theory is included at the end of the chapter.

**THE PLASMA PHYSICS INTERFACES**

The Plasma Reactor Interfaces chapter describes three of the Plasma Module multiphysics interfaces. The Capacitively Coupled Plasma Interface is for studying discharges that are sustained by a time-varying electrostatic field. The DC Discharge Interface is for studying discharges that are sustained by a static electric field and secondary electron emission. Townsend coefficients can be used instead of rate coefficients for electron source terms. The Inductively Coupled Plasma Interface is for studying discharges that are sustained by induction currents. The induction currents are solved for in the frequency domain. The electron heating due to the induction currents is automatically handled by the software. The 3D models require the AC/DC Module. The underlying theory for each interface is included at the end of the chapter. The Microwave Plasma Interface requires the RF Module, and this chapter describes this multiphysics interface. The physics interface studies discharges that are sustained by electromagnetic waves (wave-heated discharge). Heating of the electrons due to their interaction with the electromagnetic waves is automatically handled by the software. The electromagnetic waves are solved for in the frequency domain. The underlying theory is included at the end of the chapter.
Data Required for Plasma Modeling

Modeling of low-temperature plasmas is not only difficult because of the large number of physical processes occurring but also because of the amount of data that needs to be supplied to a model. This chapter gives an overview of the data you need to assemble before attempting to model a plasma.

In this chapter:

- Data Requirements
- Importing Collision Cross-Section Data
Data Requirements

This section gives an overview of the data to be assembled before attempting to model a plasma.

One of the main difficulties is to find a complete and physically correct chemical mechanism for the plasma of interest. This can involve just a handful of reactions and species (as for argon), or in the case of molecular gases there can be hundreds of reactions and tens of hundreds of species. Often the chemical mechanism can be found from a literature search, but if it is a unique plasma chemistry then the chemical mechanism is likely unknown. The only option is to find a plasma chemistry that exhibits similar properties to your specific application and use that as a reference.

The following sections guide you through the data need for each of the features which make up a plasma model.

- Electron Impact Reactions
- Reaction
- Surface Reaction
- Species

Electron Impact Reactions

For each electron impact reaction, the reaction formula is the first piece of information that is required. Most published papers involving the numerical modeling of plasmas include a table of the reactions which make up the plasma chemistry.

Once the formula is entered you need to supply some data to indicate the dependency of the reaction rate on the electron energy. The most common way of accomplishing this is to specify cross-section data for each of the electron impact reactions. The cross-section data can be hard to find or not even exist. Cross-section data is available for most of the common gases. Some useful resources for cross-section data are available at the following links:

- www.lxcat.laplace.univ-tlse.fr/cross_sec_download.php
If cross-section data is not available then the rate coefficient can be specified with a constant value, an Arrhenius expression, or by a lookup table. In the case of an Arrhenius expression, the Arrhenius coefficients must be specified. If you want to use lookup tables for the rate coefficient then you need to load in a table of rate or Townsend coefficient versus mean electron energy.

Depending on the type of electron impact collision, the following data is also required:

- The mass ratio of the electron to the target species for elastic collisions.
- The energy loss (in eV) for inelastic collisions.
- The ratio of statistical weights between the target and produced species if a detailed balance is required.

**Reaction**

For gas phase reactions, the forward rate constant using either Arrhenius coefficients or numeric value data is required. If the reaction is reversible then enter the reverse rate constant in the same way.

**Surface Reaction**

For surface reactions the following data is required:

- The forward sticking or rate coefficient, which can either be a numeric value or specified in terms of Arrhenius parameters as a function of the surface temperature.
- For first-order reactions, the total surface site concentration is required.
- For surface reactions that result in emission of secondary electrons, the secondary emission coefficient and mean energy of the secondary electrons is required.
Species

For each of the heavy species the following information is required:

- The molecular weight of the species
- The potential characteristic length of the species; required to compute the correct diffusivity and mobility
- The potential energy minimum of the species; required to compute the correct diffusivity and mobility

In cases where you are interested in solving for the neutral gas temperature, the following additional information is required:

- The species molar enthalpy, entropy, and specific heat, which can be entered directly as a function of temperature or by using *NASA polynomials*
- In the case of electronically excited species or ions, the properties of the ground state species can be entered, and an additional contribution to the species enthalpy can also be entered

The Plasma Module provides predefined transport and thermodynamic data for the following species:

<table>
<thead>
<tr>
<th>GAS</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helium</td>
<td>He</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
</tr>
<tr>
<td>Krypton</td>
<td>Kr</td>
</tr>
<tr>
<td>Xenon</td>
<td>Xe</td>
</tr>
<tr>
<td>Carbon</td>
<td>C</td>
</tr>
<tr>
<td>Carbon hydride</td>
<td>CH</td>
</tr>
<tr>
<td>Methylene</td>
<td>CH2</td>
</tr>
<tr>
<td>Methyl radical</td>
<td>CH3</td>
</tr>
<tr>
<td>Methane</td>
<td>CH4</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO2</td>
</tr>
<tr>
<td>Atomic fluorine</td>
<td>F</td>
</tr>
<tr>
<td>Fluorine</td>
<td>F2</td>
</tr>
</tbody>
</table>
The following surface species properties are also predefined:

**TABLE 2-2: TABLE OF SURFACE SPECIES WITH PREDEFINED PHYSICAL AND THERMODYNAMIC DATA**

<table>
<thead>
<tr>
<th>NAME</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon</td>
<td>Si</td>
</tr>
<tr>
<td>Silicon hydride</td>
<td>SiH</td>
</tr>
<tr>
<td>Silicon dioxide</td>
<td>SiO2</td>
</tr>
</tbody>
</table>
Importing Collision Cross-Section Data

To facilitate the modeling process, all multiphysics interfaces and the Boltzmann Equation, Two-Term Approximation interface can import sets of collision cross sections from file. This section details the file format required and has these topics:

- Cross-Section Data File Format
- The File Format
- Reference for the Plasma Module Cross-Section Data Requirements

Cross-Section Data File Format

IMPORyNG CROSS SECTIONS
The file format used to import cross-section data is almost the same as the format proposed by Hagelaar in Ref. 1. The best way to get the cross-section data in the correct format is to modify the file \texttt{Ar\_xsecs.txt} which is available in the Plasma Module model library folder.

For each electron impact reaction, the \textit{lookup table of} electron energy (eV) versus collision cross section (m$^2$) allows electron transport properties and source coefficients to be computed. As an example, a set of collision cross sections for oxygen are shown
in Figure 2-1.

![Figure 2-1: Plot of a set of collision cross sections for molecular oxygen. There are 16 collisions in total.](image)

**The File Format**

Cross-section data must be specified using the following format:

```
1st line
2nd line
3rd line
4th line
```

<table>
<thead>
<tr>
<th>energy data (eV)</th>
<th>Collision cross section (m²)</th>
</tr>
</thead>
</table>

1. 1st line: Keyword in capitals indicating the type of the collision. Possible collision types are ELASTIC, EXCITATION, IONIZATION, and ATTACHMENT. Note the use of capital letters.

2. 2nd line: Reaction formula. This formula carries over to the COMSOL Multiphysics GUI so that whatever is entered here appears in the Formula field. The formula must be separated by a => sign.

3. 3rd line: For elastic collisions, the ratio of the electron mass to the target particle mass. For attachment, the 3rd line is 0 (zero). For ionization, the threshold energy
in eV. For excitation there are three (3) numbers separated by a space. The first number is the excitation energy (eV). The second number is the ratio of statistical weights of the final state to the initial state. The third number is a flag that determines whether or not a detailed balance is used. Use a 1 to construct a detailed balance and 0 otherwise.

4 4th line: Two unit conversion factors by which the columns of data are multiplied.

Table of the cross section as a function of energy. The table starts and ends by a line of dashes ‘- - - - -’ (at least five), and has otherwise two numbers per line: the energy in eV and the cross section in m$^2$. The table does not need to follow the other lines immediately; that is, user comments such as reference information can be included above the table.

Here are some examples for the types of collisions available:

ELASTIC
e+O2=>e+O2
1.71e-5
1.0 1.0

-------------------------------
0.000000e+000 3.500000e-021
.
.
-------------------------------
ATTACHMENT
e+O2=>O+O-
0
1.0 1.0

-------------------------------
5.800000e-002 2.220446e-036
.
.
-------------------------------
EXCITATION
e+O2=>e+O2b1s
1.6270 5 1
1.0 1.0

-------------------------------
1.627000e+000 2.220446e-036
.
.
-------------------------------
IONIZATION

e+O2+->2e+O2+

12.0600

1.0 1.0

---------------------------------

1.20600e+001 2.220446e-036

Reference for the Plasma Module Cross-Section Data Requirements

The AC/DC Branch

This chapter describes the interfaces available with the Plasma Module under the AC/DC branch (_visual_icon) when adding a physics interface. Use the Electrostatics interface to compute the electrostatic field in the plasma caused by separation of space charge between the electrons and ions. This module enhances the interface included with the basic COMSOL Multiphysics® license. Use the Electrical Circuit interface to add an external electrical circuit to the plasma model.

In this chapter:

- The Electrostatics Interface
- The Electrical Circuit Interface
- Theory of Electric Fields
- Theory for the Electrostatics Interface
- Theory for the Electrical Circuit Interface
- Connecting to Electrical Circuits
- Spice Import
The Electrostatics Interface

The Electrostatics (es) interface ( ), found under the AC/DC branch ( ) when adding a physics interface, is used to compute the electric field, the electric displacement field and potential distributions in dielectrics under conditions where the electric charge distribution is explicitly prescribed. The formulation is stationary but for use together with other physics, also 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—Charge Conservation, 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 from the context menu.

Interface Identifier

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

The default identifier (for the first interface in the model) is es.

Domain Selection

The default setting is to include All domains in the model to define the electric potential and the equations that describe the potential field for dielectrics. To choose specific domains, select Manual from the Selection list.
**THICKNESS**

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 models. See also Change Cross-Section.

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 models. See also Change Thickness (Out-of-Plane).

**DISCRETIZATION**

To display this section, click the Show button ( ) and select Discretization. Select an element order for the Electric potential—Linear, Quadratic (the default), Cubic, Quartic, or (in 2D only) Quintic. Specify the Value type when using splitting of complex variables—Real or Complex (the default).

**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 electric potential field 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.

- Show More Physics Options
- Domain, Boundary, Edge, Point, and Pair Nodes for the Electrostatics Interface
- Theory for the Electrostatics Interface

**Electric Sensor**: model 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

\[ \mathbf{n} \cdot [(\varepsilon_0 \nabla \mathbf{V} - \mathbf{P})_1 - (\varepsilon_0 \nabla \mathbf{V} - \mathbf{P})_2] = -\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0 \]

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 3-1 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.
Table 3-1 lists the interior and exterior boundaries available with this physics interface. It also includes edge, point, and pair availability.

<table>
<thead>
<tr>
<th>NODE</th>
<th>INTERIOR</th>
<th>EXTERIOR</th>
<th>ALSO AVAILABLE FOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Change Cross-Section</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Change Thickness (Out-of-Plane)</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Charge Conservation</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Dielectric Shielding</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Distributed Capacitance</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Electric Displacement Field</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Electric Potential</td>
<td>x</td>
<td></td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>Electrostatic Point Dipole</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>External Surface Charge Accumulation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Floating Potential</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Ground</td>
<td>x</td>
<td></td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>Periodic Condition</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Surface Charge Accumulation</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Surface Charge Density</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Terminal</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
</tbody>
</table>

Table 3-1: Interior and exterior boundary conditions (including edge, point, and pair availability) for the Electrostatics Interface.
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.

Domain Selection

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically set up and is the same as for the physics interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains to define the electric potential and the equation based on Gauss' law that describes the potential field or select All domains as required.

Model Inputs

This section contains field variables that appear as model inputs, if the current settings include such model inputs. By default, this section is empty.

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

<table>
<thead>
<tr>
<th>NODE</th>
<th>INTERIOR</th>
<th>EXTERIOR</th>
<th>ALSO AVAILABLE FOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thin Low Permittivity Gap</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Zero Charge (the default)</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
</tbody>
</table>

For axisymmetric models, 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:
- Continuity on Interior Boundaries
- Identity and Contact Pairs

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.
change as functions of material strain, material orientation and other variables evaluated in a material reference configuration (material frame). Select Non-solid 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.

**COORDINATE SYSTEM SELECTION**

The Global coordinate system is selected by default. The Coordinate system list contains any additional coordinate systems that the model includes.

**ELECTRIC FIELD**

Select a Constitutive relation 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.

Select:

- **Relative permittivity** (the default) to use the constitutive relation \( D = \varepsilon_0 \varepsilon_r E \). Then the default is to take the Relative permittivity \( \varepsilon_r \) (dimensionless) values From material. If User defined is selected, select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. The default is 1.

- **Polarization** to use the constitutive relation \( D = \varepsilon_0 E + P \). Then enter the components based on space dimension for the Polarization vector \( P \) (SI unit: C/m\(^2\)). The defaults are 0 C/m\(^2\).

- **Remanent electric displacement** to use constitutive relation \( D = \varepsilon_0 E + D_r \), where \( D_r \) is the remanent displacement (the displacement when no electric field is present). Then the default is to take the Relative permittivity \( \varepsilon_r \) (dimensionless) values From material. If User defined is selected, select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. Then enter the components based on space dimension for the Remanent electric displacement \( D_r \) (SI unit: C/m\(^2\)). The defaults are 0 C/m\(^2\).

**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.
**DOMAIN SELECTION**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically set up and is the same as for the physics interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

**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 $\rho$, which appears on the right-hand side of the equation that the physics interface defines.

**DOMAIN SELECTION**

From the Selection list, choose the domains to define.

**SPACE CHARGE DENSITY**

Enter a value or expression for the Space charge density $\rho_q$ (SI unit: C/m$^3$). The default is 0 C/m$^3$.

*Zero Charge*

The Zero Charge node adds the condition that there is zero charge on the boundary so that $n \cdot D = 0$. 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.

**BOUNDARY SELECTION**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically set up and is the same as for the physics interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific boundaries or select All boundaries as required.
PAIR SELECTION

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

Ground

The Ground node is the default boundary condition and 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 models) or Points (2D and 3D models) submenus. For 2D axisymmetric models, it can be applied on the Symmetry axis.

BOUNDARY, EDGE, OR POINT SELECTION

From the Selection list, choose the geometric entity (boundaries, edges, or points) to define.

| 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. |

PAIR SELECTION

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

CONSTRAINT SETTINGS

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

To Apply reaction terms on all dependent variables, select All physics (symmetric).

Otherwise, select Current physics (internally symmetric) or Individual dependent variables to restrict the reaction terms as required. Select the Use weak constraints check box to replace the standard constraints with a weak implementation.
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 models) or Points (2D and 3D models) submenus. For 2D axisymmetric models, it can be applied on the symmetry axis.

Boundary, Edge, or Point Selection

From the Selection list, choose the geometric entities (boundaries, edges, or points) to define.

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.

Pair Selection

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

Electric Potential

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

Circuit Settings

Theory for the Capacitively Coupled Plasma Interface

Select the Circuit type—None (the default), Series RC circuit, Ballast resistor, or Blocking capacitor. If None is selected, no external circuit is added.
**Series RC Circuit**
If **Series RC circuit** is selected, enter a value or expression for the **Ballast resistor** $R_b$ (SI unit: $\Omega$) and **Blocking capacitance** $C_b$ (SI unit: F). The defaults are 1000 $\Omega$ and 1 pF, respectively.

- This option is typically used for metallic electrodes in DC discharges. The presence of the external circuit prevents the discharge from arcing. If arcing begins to occur the solver tends to fail and the ballast resistor value should be increased. The presence of the blocking capacitor also helps when solving by ramping up the applied potential from zero over a finite period of time.

**Ballast Resistor**
If **Ballast resistor** is selected, enter a value or expression for the **Ballast resistor** $R_b$ (SI unit: $\Omega$). The default is 1000 $\Omega$.

- The presence of the ballast resistor reduces the likelihood that the discharge arcs. However, it is recommended that the **Series RC circuit** be chosen in preference to this one.

**Blocking Capacitor**
If **Blocking capacitor** is selected, enter a value or expression for the **Blocking capacitance** $C_b$ (SI unit: F). The default is 1 pF.

- This option is typically used when modeling capacitively coupled plasmas, since these typically operate with a blocking capacitor between the power supply and the electrodes.

For 1D models, enter a value for the **Electrode surface area** $A_s$ (SI unit: $m^2$). The default is 0.01 $m^2$. This value is used to compute the total amount of electrical current flowing into the electrode due to the time varying displacement field and flow of charged particles.

**Constraint Settings**
To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. To **Apply reaction terms on** all dependent variables, select **All physics (symmetric)**.
Otherwise, select **Current physics (internally symmetric)** or **Individual dependent variables** to restrict the reaction terms as required. Select the **Use weak constraints** check box to replace the standard constraints with a weak implementation.

**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 \(\rho_s\) at an outer boundary or at an interior boundary between two nonconducting media. Also right-click to add a **Harmonic Perturbation** subnode.

**BOUNDARY SELECTION**

From the **Selection** list, choose the boundaries to define.

**PAIR SELECTION**

If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**SURFACE CHARGE DENSITY**

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

---

Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the **COMSOL Multiphysics Reference Manual**

---

**External Surface Charge Accumulation**

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

\[-\mathbf{n} \cdot \mathbf{D} = \rho_s\]

where \(\rho_s\) 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.

**Boundary Selection**

From the **Selection** list, choose the boundaries to define.

**Pair Selection**

If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**External Surface Charge Accumulation**

Enter values or expressions for the **Normal ion current density** $\mathbf{n} \cdot \mathbf{J}_i$ (SI unit: A/m$^2$) and the **Normal electron current density** $\mathbf{n} \cdot \mathbf{J}_e$ (SI unit: A/m$^2$). The defaults are 0 A/m$^2$ for both.

_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.

**Boundary Selection**

From the **Selection** list, choose the boundaries to define.

**Pair Selection**

If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**Coordinate System Selection**

The **Global coordinate system** is selected by default. The **Coordinate system** list contains any additional coordinate systems that the model includes.

**Electric Displacement Field**

Enter the coordinates of the **Boundary electric displacement field** $\mathbf{D}_0$ (SI unit: C/m$^2$), the defaults are 0 C/m$^2$. 
**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** subnode. With this subnode the boundaries which constitute the source and destination surfaces can be manually specified. To add the subnode, right-click the **Periodic Condition** node and select **Destination Selection**.

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

**Boundary Selection**

From the **Selection** list, choose the boundaries to define.

When using non conforming 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.

**Periodic Condition**

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

**Constraint Settings**

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

To **Apply reaction terms** on all dependent variables, select **All physics (symmetric)**.

Otherwise, select **Current physics (internally symmetric)** or **Individual dependent**.
variables to restrict the reaction terms as required. Select the **Use weak constraints** check box to replace the standard constraints with a weak implementation.

In the *COMSOL Multiphysics Reference Manual*:
- Periodic Condition and Destination Selection
- Periodic Boundary Conditions

**Thin Low Permittivity Gap**

Use the **Thin Low Permittivity Gap** node

\[
\mathbf{n} \cdot \mathbf{D}_1 = \frac{\varepsilon_0 \varepsilon_r}{d_s} (V_1 - V_2)
\]

\[
\mathbf{n} \cdot \mathbf{D}_2 = \frac{\varepsilon_0 \varepsilon_r}{d_s} (V_2 - V_1)
\]

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

**BOUNDARY SELECTION**

From the **Selection** list, choose the boundaries to define.

**PAIR SELECTION**

If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**THIN LOW PERMITTIVITY GAP**

The default is to take the **Relative permittivity** \(\varepsilon_r\) (dimensionless) values From material. Select **User defined** to enter a different value or expression. Enter a **Surface thickness** \(d_s\) (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 $\rho_s$ is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{d\ell} = n \cdot J_i + n \cdot J_e$$

where $n \cdot J_i$ is the normal component of the total ion current density on the wall and $n \cdot J_e$ is the normal component of the total electron current density on the wall.

**BOUNDARY SELECTION**
From the **Selection** list, choose the boundaries to define.

**SURFACE CHARGE ACCUMULATION**
Enter the values or expressions for the **Normal ion current density** $n \cdot J_i$ (SI unit: A/m$^2$) and the **Normal electron current density** $n \cdot J_e$ (SI unit: A/m$^2$).  

---

### 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 $\varepsilon_r$ that shields the electric field:

$$n \cdot D = -\nabla \cdot \epsilon_0 \epsilon_r d_s \nabla V$$

---

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

**BOUNDARY OR EDGE SELECTION**
From the **Selection** list, choose the geometric entity (boundaries or edges) to define.

**PAIR SELECTION**
If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.
ELECTRIC SHIELDING
The default is to take the Relative permittivity \( \varepsilon_r \) (dimensionless) values From material. It takes it from the adjacent domains if not explicitly defined. If User defined is selected, select Isotropic, Diagonal, Symmetric, or Anisotropic 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 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. The Terminal node also enables the computation of the lumped parameters of the system, such as capacitance.

BOUNDARY SELECTION
From the Selection list, choose the boundaries to model as terminals connected to external circuits, an external voltage, or supporting a fixed charge.

PAIR SELECTION
If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

TERMINAL
Specify the terminal properties. To indicate which boundaries belong to the same terminal, enter the same name in the Terminal name field. The Terminal name should be numeric for sweeps to work properly.

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

- Charge to enter the total charge \( Q_0 \) (SI unit: C). The default is 0 C for a floating electrode.
- Voltage to enter an electric potential \( V_0 \) (SI unit: V). The default is 1 V.
• **Circuit** to specify a terminal connected to an external circuit. The Terminal node provides a current-voltage characteristic to the circuit element.

| The Electrical Circuit Interface requires a current from the Terminal, so the Circuit terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge.

| The Circuit type cannot be used together with a terminal sweep.

| Studies and Solvers in the COMSOL Multiphysics Reference Manual

• **Terminated** to connect the terminal to an impedance that might represent a load or a transmission line. When Terminated is selected, the scattering parameters (S-parameters) are computed.
  - Enter a **Terminal power** \( P_0 \) (SI unit: W) 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**. If **Physics interface** is selected, the **Reference impedance** \( Z_{\text{ref}} \) defined on the interface settings window under Sweep Settings is used. If **User defined** is selected, enter a specific impedance \( Z_{\text{ref}} \) (SI unit: \( \Omega \)) for this terminal. The default is 50 \( \Omega \).

**CONSTRAINT SETTINGS**

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. To **Apply reaction terms on** all dependent variables, select **All physics (symmetric)**. Otherwise, select **Current physics (internally symmetric)** or **Individual dependent variables** to restrict the reaction terms as required. Select the **Use weak constraints** check box to replace the standard constraints with a weak implementation.

**Floating Potential**

The **Floating Potential** node is used when modeling a metallic electrode at floating potential. The electrode might have a charge \( Q_0 \) deposited on it, or can be connected to an electrical circuit.
BOUNDARY SELECTION

From the Selection list, choose the boundaries to define. For the Piezoresistivity, Shell interface, select edges instead of boundaries.

PAIR SELECTION

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

FLOATING POTENTIAL

The default Floating potential identifier cannot be edited, it is provided as an aid in identifying associated potential variables in postprocessing. The Floating potential group check box controls how potentials are assigned to boundary segments in the feature’s Boundary Selection. If this check box is not selected, a single potential is applied to all boundaries in the selection. If the check box is selected, each group of contiguous boundary segments within the selection is given a unique potential. This simplifies the setup of models with many floating electrodes. The potential variables are then available in postprocessing as a vector variable. Only the “zero total charge” setting is available for the floating potential group.

The following option is not available if the Floating potential group check box controls how potentials is selected. Select a specification for the Electric charge—choose User defined to specify a Charge $Q_0$ (SI unit: C) deposited on the surface. The default is 0 C. Choose Circuit to connect the floating potential to an Electrical Circuit.

The Electrical Circuit Interface requires a current from the Floating Potential, so the Circuit terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge.

CONSTRAINT SETTINGS

To display this section, click the Show button ( ) and select Advanced Options. To Apply reaction terms on all dependent variables, select All (symmetric). Otherwise, select Current (internally symmetric) or Individual dependent variables to restrict the reaction terms as required.
**Distributed Capacitance**

The Distributed Capacitance node adds a distributed capacitance boundary condition according to the following equations for exterior boundaries (left) and interior boundaries (right):

\[
\mathbf{n} \cdot \mathbf{D} = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s} \quad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s}
\]

**Boundary Selection**

From the Selection list, choose the boundaries define.

**Pair Selection**

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**Distributed Capacitance**

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

**Line Charge**

For 3D models, use the Line Charge node to specify line charges along the edges of a geometry. Also right-click to add a Harmonic Perturbation subnode.
**EDGE SELECTION**

From the Selection list, choose the edges to define.

⚠️ 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)
- Line Charge (Out-of-Plane)
- Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the COMSOL Multiphysics Reference Manual

For 2D axisymmetric models, use the Line Charge (on Axis) node to specify line charges along the symmetry axis. Also right-click to add a Harmonic Perturbation subnode.

**BOUNDARY SELECTION**

From the Selection list, choose the boundaries to define.

**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
- Line Charge (Out-of-Plane)
- Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the COMSOL Multiphysics Reference Manual
Line Charge (Out-of-Plane)

For 2D and 2D axisymmetric models, points are selected and this is the same as a line out-of-plane. Also right-click to add a Harmonic Perturbation subnode.

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

**POINT SELECTION**

From the Selection list, choose the points to define.

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
- Line Charge (on Axis)
- Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the COMSOL Multiphysics Reference Manual

Point Charge

The Point Charge node adds a point source to 3D models. The point charge represents an electric displacement field flowing out of the point. Also right-click to add a Harmonic Perturbation subnode.
**POINT SELECTION**

From the *Selection* list, choose the points to define.

---

⚠️ 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)**
- **Line Charge (Out-of-Plane)**
- **Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis** in the *COMSOL Multiphysics Reference Manual*

---

*Point Charge (on Axis)*

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The **Point Charge (on Axis)** node adds a point source to 2D axisymmetric models. The point charge represents an electric displacement field flowing out of the point. Also right-click to add a **Harmonic Perturbation** subnode.

---

**POINT SELECTION**

From the *Selection* list, choose the points to define.

---

⚠️ 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 axis. This source represents an electric displacement field flowing out of the point. The default is 0 C.

- **Point Charge**
- **Line Charge (Out-of-Plane)**
- **Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis** in the COMSOL Multiphysics Reference Manual

**Change Cross-Section**

This node is available with 1D models. This setting overrides the global Thickness setting made in any physics interface that uses this feature.

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

**DOMAIN OR BOUNDARY SELECTION**

From the Selection list, choose the geometric entity (domains or boundaries) to define.

**PAIR SELECTION**

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**CHANGE CROSS-SECTION**

Enter a value or expression for the Cross-section area \( A \) (SI unit: m\(^2\)). The default value of 1 unit length 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 models.

For 2D models, see Change Thickness (Out-of-Plane).
**Change Thickness (Out-of-Plane)**

This node is available for 2D models. This setting overrides the global Thickness setting made in any physics interface that uses this node.

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

**DOMAIN OR BOUNDARY SELECTION**

From the Selection list, choose the geometric entity (domains or boundaries) to define.

**PAIR SELECTION**

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**CHANGE THICKNESS (OUT-OF-PLANE)**

Enter a value or expression for the Out-of-plane thickness \( d \) (SI unit: m). 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 models.

For 1D models, see Change Cross-Section.

**Electrostatic Point Dipole**

Add an Electrostatic Point Dipole node to 3D and 2D models. Also right-click to add a Harmonic Perturbation subnode.

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.

**POINT SELECTION**

From the **Selection** list, choose the points (also on axis) to define.

**ELECTROSTATIC POINT DIPOLE**

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

- If **Magnitude and direction** is selected, enter coordinates for the **Electric dipole moment direction** \( \mathbf{n}_p \) (dimensionless) and the **Electric dipole moment, magnitude** \( p \) (SI unit: C·m).
- If **Electric dipole moment** is selected, enter coordinates for the **Electric dipole moment** \( p \) (SI unit: C·m).

---

Harmonic Perturbation, Prestressed Analysis, and Small-Signal Analysis in the *COMSOL Multiphysics Reference Manual*
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 interface is added, it adds a default Ground Node feature and associates that with node zero in the electrical circuit.

DEVICE NAMES

Each circuit component has an associated Device name, which is constructed from a prefix identifying the type of the device and a string. The string can be specified in the feature’s Settings window. The Device name is used to identify variables defined by the component, and for the SPICE import functionality.

INTERFACE IDENTIFIER

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

The default identifier (for the first interface in the model) is cir.

Circuit nodes are nodes in the electrical circuit (electrical nodes) and should not be confused with nodes in the Model Builder tree of COMSOL Multiphysics. Circuit node names are not restricted to numerical values but can be arbitrary character strings.
CHAPTER 3: THE AC/DC BRANCH

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 $1 \times 10^{12}$ Ω.

The following are available from the Physics ribbon toolbars (Windows users), Physics contextual toolbar (Mac and Linux users), or for any user, right-click to select it from the context menu for the interface:

- Theory for the Electrical Circuit Interface
- Connecting to Electrical Circuits

In general, click a button on the Physics toolbar, no matter what operating system you are using.

- Ground Node
- Resistor
- Capacitor
- Inductor
- Voltage Source
- Current Source
- Voltage-Controlled Voltage Source
- Voltage-Controlled Current Source
- Current-Controlled Voltage Source
- Current-Controlled Current Source
- Subcircuit Definition
- Subcircuit Instance
- NPN BJT
- n-Channel MOSFET
- Diode
- External I vs. U
- External U vs. I
- External I-Terminal
- SPICE Circuit Import

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.
GROUN D  C O N N E C T I O N
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).

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

D E V I C E  N A M E
Enter a Device name for the resistor. The prefix is R.

N O D E  C O N N E C T I O N S
Set the two Node names for the connecting nodes for the resistor.

D E V I C E  P A R A M E T E R S
Enter the Resistance of the resistor.

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

D E V I C E  N A M E
Enter a Device name for the capacitor. The prefix is C.

N O D E  C O N N E C T I O N S
Set the two Node names for the connecting nodes for the capacitor.

D E V I C E  P A R A M E T E R S
Enter the Capacitance of the capacitor.

Inductor
The Inductor ( ) feature connects an inductor between two nodes in the electrical circuit.
DEVICE NAME
Enter a Device name for the inductor. The prefix is L.

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.

DEVICE NAME
Enter a Device name for the voltage source. The prefix is V.

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 DC-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 DC-source, the Voltage $V_{src}$ (default value: 1 V). DC-sources are active in Stationary and Time-Dependent studies.

• For an AC-source: the Voltage $V_{src}$ (default value: 1 V) and the Phase $\Theta$ (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 $\Theta$ (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: 0 s), the Rise time $t_r$ and Fall time $t_f$ (default values: 0 s), the Pulse width $p_w$ (default value: 1 µs), and the Period $T_{per}$ (default value: 2 µs). 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 (\( \text{Current Source} \)) feature connects a current source between two nodes in the electrical circuit.

**Device Name**

Enter a Device name for the current source. The prefix is I.

**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 DC-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 DC-source, the Current \( i_{\text{src}} \) (default value: 1 A). DC-sources are active in Stationary and Time-Dependent studies.
- For an AC-source: the Current \( i_{\text{src}} \) (default value: 1 A) and the Phase \( \Theta \) (default value: 0 rad). AC-sources are active in Frequency Domain studies only.
- For a sine source: the Current \( i_{\text{src}} \) (default value: 1 A), the Offset \( i_{\text{off}} \) (default value: 0 A), the Frequency (default value: 1 kHz), and the Phase \( \Theta \) (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 \( i_{\text{src}} \) (default value: 1 A), the Offset \( i_{\text{off}} \) (default value: 0 A), 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 µs), and the Period $T_{per}$ (default value: 2 µs).
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.

**DEVICE NAME**
Enter a Device name for the voltage-controlled voltage source. The prefix is E.

**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**
Enter the voltage Gain. The resulting voltage is this number multiplied by the control voltage.

**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.

**DEVICE NAME**
Enter a Device name for the voltage-controlled current source. The prefix is G.
**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**

Enter the source **Gain** (SI units: S). The resulting current is this number multiplied by the control voltage. It represents the transconductance of the source.

*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.

**DEVICE NAME**

Enter a **Device name** for the current-controlled voltage source. The prefix is H.

**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**

Enter the voltage **Gain** and select the **Device** whose current is taken as the control current. The resulting voltage is this number multiplied by the control current through the named **Device** (any two-pin device). Thus it formally has the unit of resistance.

*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.

**DEVICE NAME**

Enter a **Device name** for the current-controlled current source. The prefix is F.
**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**

Enter the current Gain and select the Device whose current is taken as the control current. The resulting current is this number multiplied by the control current through the Device.

**Subcircuit Definition**

The Subcircuit Definition ( ) feature is used to define subcircuits. From the Physics toolbar, add a Subcircuit Definition node to add the circuit components constituting the subcircuit. Also right-click to Rename the node.

**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.

**Subcircuit Instance**

The Subcircuit Instance ( ) feature is used to refer to defined subcircuits.

**DEVICE NAME**

Enter a Device name for the subcircuit instance. The prefix is X.

**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.

**Spice Import**
**NPN BJT**

The **NPN BJT** device model is a large-signal model for an NPN bipolar junction transistor (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.

**DEVICE NAME**

Enter a **Device name** for the BJT. The prefix is Q.

**NODE CONNECTIONS**

Specify three **Node names** for the connection nodes for the NPN BJT device. These represent the **collector**, **base**, and **emitter** nodes, respectively. If the ground node is involved, the convention is to use 0 (zero) for this but it is allowed to have more than one ground node provided it has been given a unique node name.

**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.

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The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits.

For an explanation of the **Model Parameters** see **NPN Bipolar Transistor**.

---

**n-Channel MOSFET**

The **n-Channel MOSFET** device model is a large-signal model for an n-Channel MOS transistor (MOSFET). 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 parameters for this MOSFET model. For any particular make of MOSFET, the device manufacturer should be the primary source of information.

**DEVICE NAME**

Enter a **Device name** for the MOSFET. The prefix is M.
CHAPTER 3: THE AC/DC BRANCH

NODE CONNECTIONS
Specify four **Node names** for the connection nodes for the *n-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.

---

**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.

DEVICE NAME
Enter a **Device name** for the diode. The prefix is D.

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 *n-Channel MOS Transistor*.
**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) as a 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.

**DEVICE NAME**
Enter a **Device name** for the External I vs. U node.

**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 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 for 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 `cirn.IvsUm_i`, where `cirn` is the tag of the Electrical Circuit interface node and `IvsUm` is the tag of the **External I vs. U** node. The mentioned tags are typically displayed within curly braces {} in the Model Builder tree.

Component Couplings in the **COMSOL Multiphysics Reference Manual**
**External U vs. I**

The External U vs. I (\[\text{eq:uvsim} \]) feature connects an arbitrary current measurement (for example, from another) as a 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.

**DEVICE NAME**

Enter a Device name for the External U vs. I node.

**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 \(\text{cirn.UvsIm} \_v\), where \(\text{cirn}\) is the tag of the Electrical Circuit interface node and \(\text{UvsIm}\) is the tag of the External U vs. I node. The mentioned tags are typically displayed within curly braces \(\{}\) in the Model Builder tree.

**External I-Terminal**

The External I-Terminal (\[\text{eq:etterm} \]) feature connects an arbitrary voltage-to-ground measurement (for example, a circuit terminal boundary from another 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.

**DEVICE NAME**

Enter a **Device name** for the External I-terminal.

**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.

Except for 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 cirn.termIm_i, where cirn is the tag of the Electrical Circuit interface node and termIm is the tag of the **External I-Terminal** node. The mentioned tags are typically displayed within curly braces {} in the Model Builder tree.

Component Couplings in the **COMSOL Multiphysics Reference Manual**

**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.
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 for more details on the supported SPICE commands.
**Theory of Electric Fields**

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. This section is a brief introduction to **Charge Relaxation Theory**.

**Charge Relaxation Theory**

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**

\[ \mathbf{J} = \sigma \mathbf{E} \]

the **equation of continuity**

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0 \]

and **Gauss’ law**

\[ \nabla \cdot (\varepsilon \mathbf{E}) = \rho \]

By combining these, one can deduce the following differential equation for the space charge density in a homogeneous medium

\[ \frac{\partial \rho}{\partial t} + \frac{\sigma}{\varepsilon} \rho = 0 \]

This equation has the solution

\[ \rho(t) = \rho_0 e^{-t/\tau} \]

where
is called the charge relaxation time. For a good conductor like copper, $\tau$ 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 3-2 below,

<table>
<thead>
<tr>
<th>CASE</th>
<th>INTERFACE</th>
<th>STUDY TYPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau \gg t$</td>
<td>Electrostatics</td>
<td>Stationary</td>
</tr>
<tr>
<td>$\tau \ll t$</td>
<td>Electric Currents</td>
<td>Stationary</td>
</tr>
<tr>
<td>$\tau \approx t$</td>
<td>Electric Currents</td>
<td>Time Dependent or Frequency Domain</td>
</tr>
</tbody>
</table>

**FIRST CASE:** $t \gg \tau$

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, and 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 $E = -\nabla V$. Using this together with the constitutive relation $D = \varepsilon_0 E + P$ between $D$ and $E$, you can rewrite Gauss’ law as a variant of Poisson’s equation

$$-\nabla \cdot (\varepsilon_0 \nabla V - P) = \rho$$

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.
That typically involves either prescribing the charge dynamics or coupling a separate formulation for this.

**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 than above of Ohm’s law states that

\[
\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}^e
\]

where \( \mathbf{J}^e \) is an externally generated current density. The static form of the equation of continuity then reads

\[
\nabla \cdot \mathbf{J} = -\nabla \cdot (\sigma \nabla V - \mathbf{J}^e) = 0
\]

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.

Such separate charge transport formulations can be found in the Plasma Module and the Chemical Reaction Engineering Module.
Theory for the Electrostatics Interface

The Electrostatics Interface is available for 3D, 2D in-plane, and 2D axisymmetric models. 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 is short compared to the charge relaxation time and that 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.

Electrostatics Equations

Under static conditions the electric potential, $V$, is defined by the relationship:

$$E = -\nabla V$$

Combining this equation with the constitutive relationship $D = \varepsilon_0 E + P$ between the electric displacement $D$ and the electric field $E$, it is possible to represent Gauss' law as the following equation:

$$-\nabla \cdot (\varepsilon_0 \nabla V - P) = \rho$$

In this equation, the physical constant, $\varepsilon_0$ (SI unit: F/m) is the permittivity of vacuum, $P$ (SI unit: C/m$^2$) is the electric polarization vector, and $\rho$ (SI unit: C/m$^3$) 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, $E$, is tangential to the $xy$-plane. With this symmetry, the same equation is solved as in the 3D case. The interface solves the following equation where $d$ is the thickness in the $z$ direction:

$$-\nabla \cdot (\varepsilon_0 \nabla V - P) = \rho$$
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 $\phi$ 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 be solved also in a dynamic study (Time Dependent or Frequency Domain). The equation system solved, however, is 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. Using the 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, that can be used when on a static bias charge or voltage is superposed a time-harmonic perturbation.
Theory for the Electrical Circuit Interface

The Electrical Circuit Interface theory is discussed in this section:

- Electric Circuit Modeling and the Semiconductor Device Models
- NPN Bipolar Transistor
- n-Channel MOS Transistor
- Diode
- Reference for the Electrical Circuit Interface

Connecting to Electrical Circuits

Electric 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 non-ideal circuit elements are described in this section. For a more detailed account on semiconductor device modeling, see Ref. 1.

**NPN Bipolar Transistor**

*Figure 3-1* illustrates the equivalent circuit for the bipolar transistor.

*Figure 3-1: A circuit for the bipolar transistor.*

The following equations are used to compute the relations between currents and voltages in the circuit.
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.

The model parameters are listed in the table below.

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B_F )</td>
<td>100</td>
<td>Ideal forward current gain</td>
</tr>
<tr>
<td>( B_R )</td>
<td>1</td>
<td>Ideal reverse current gain</td>
</tr>
<tr>
<td>( C_{JC} )</td>
<td>0 F/m²</td>
<td>Base-collector zero-bias depletion capacitance</td>
</tr>
<tr>
<td>( C_{JE} )</td>
<td>0 F/m²</td>
<td>Base-emitter zero-bias depletion capacitance</td>
</tr>
<tr>
<td>( F )</td>
<td>0.5</td>
<td>Breakdown current</td>
</tr>
<tr>
<td>( I_{KF} )</td>
<td>Inf (A/m²)</td>
<td>Corner for forward high-current roll-off</td>
</tr>
<tr>
<td>( I_{KR} )</td>
<td>Inf (A/m²)</td>
<td>Corner for reverse high-current roll-off</td>
</tr>
</tbody>
</table>
TABLE 3-1: BIPOLAR TRANSISTOR MODEL PARAMETERS

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_S$</td>
<td>$1 \times 10^{-15} \text{ A/m}^2$</td>
<td>Saturation current</td>
</tr>
<tr>
<td>$I_{SC}$</td>
<td>$0 \text{ A/m}^2$</td>
<td>Base-collector leakage saturation current</td>
</tr>
<tr>
<td>$I_{SE}$</td>
<td>$0 \text{ A/m}^2$</td>
<td>Base-emitter leakage saturation current</td>
</tr>
<tr>
<td>$M_{JC}$</td>
<td>$1/3$</td>
<td>Base-collector grading coefficient</td>
</tr>
<tr>
<td>$M_{JE}$</td>
<td>$1/3$</td>
<td>Base-emitter grading coefficient</td>
</tr>
<tr>
<td>$N_C$</td>
<td>2</td>
<td>Base-collector ideality factor</td>
</tr>
<tr>
<td>$N_E$</td>
<td>1.4</td>
<td>Base-emitter ideality factor</td>
</tr>
<tr>
<td>$N_F$</td>
<td>1</td>
<td>Forward ideality factor</td>
</tr>
<tr>
<td>$N_R$</td>
<td>1</td>
<td>Reverse ideality factor</td>
</tr>
<tr>
<td>$R_B$</td>
<td>$0 \Omega \text{m}^2$</td>
<td>Base resistance</td>
</tr>
<tr>
<td>$R_{BM}$</td>
<td>$0 \Omega \text{m}^2$</td>
<td>Minimum base resistance</td>
</tr>
<tr>
<td>$R_C$</td>
<td>$0 \Omega \text{m}^2$</td>
<td>Collector resistance</td>
</tr>
<tr>
<td>$R_E$</td>
<td>$0 \Omega \text{m}^2$</td>
<td>Emitter resistance</td>
</tr>
<tr>
<td>$T_{NOM}$</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>$V_{AF}$</td>
<td>$\text{Inf (V)}$</td>
<td>Forward Early voltage</td>
</tr>
<tr>
<td>$V_{AR}$</td>
<td>$\text{Inf (V)}$</td>
<td>Reverse Early voltage</td>
</tr>
<tr>
<td>$V_{JC}$</td>
<td>0.71 V</td>
<td>Base-collector built-in potential</td>
</tr>
<tr>
<td>$V_{JE}$</td>
<td>0.71 V</td>
<td>Base-emitter built-in potential</td>
</tr>
</tbody>
</table>

$n$-Channel MOS Transistor

Figure 3-2 illustrates an equivalent circuit for the MOS transistor.
Figure 3-2: A circuit for the MOS transistor.

The following equations are used to compute the relations between currents and voltages in the circuit.
There are also several capacitances between the terminals

\[
C_{jbd} = C_{BD} \times \left\{ \begin{array}{ll}
& \frac{C_{gd}}{W} \quad v_{bd} < 0 \\
& \frac{C_{gs}}{W} \quad v_{bd} > 0 \\
& \frac{C_{jbd}}{W} \quad v_{bd} = 0
\end{array} \right.
\]

The model parameters are as follows:

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{BD} )</td>
<td>0 F/m</td>
<td>Bulk-drain zero-bias capacitance</td>
</tr>
<tr>
<td>( C_{GDO} )</td>
<td>0 F/m</td>
<td>Gate-drain overlap capacitance</td>
</tr>
<tr>
<td>( C_{GSO} )</td>
<td>0 F/m</td>
<td>Gate-source overlap capacitance</td>
</tr>
<tr>
<td>( F_C )</td>
<td>0.5</td>
<td>Capacitance factor</td>
</tr>
<tr>
<td>( I_S )</td>
<td>1e-13 A</td>
<td>Bulk junction saturation current</td>
</tr>
<tr>
<td>( K_P )</td>
<td>2e-5 A/V^2</td>
<td>Transconductance parameter</td>
</tr>
<tr>
<td>( L )</td>
<td>50e-6 m</td>
<td>Gate length</td>
</tr>
<tr>
<td>( M_J )</td>
<td>0.5</td>
<td>Bulk junction grading coefficient</td>
</tr>
<tr>
<td>( N )</td>
<td>1</td>
<td>Bulk junction ideality factor</td>
</tr>
</tbody>
</table>
Table 3-2: MOS Transistor Model Parameters

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_B$</td>
<td>0.75 V</td>
<td>Bulk junction potential</td>
</tr>
<tr>
<td>$R_B$</td>
<td>0 Ω</td>
<td>Bulk resistance</td>
</tr>
<tr>
<td>$R_D$</td>
<td>0 Ω</td>
<td>Drain resistance</td>
</tr>
<tr>
<td>$R_{DS}$</td>
<td>Inf (Ω)</td>
<td>Drain-source resistance</td>
</tr>
<tr>
<td>$R_G$</td>
<td>0 Ω</td>
<td>Gate resistance</td>
</tr>
<tr>
<td>$R_S$</td>
<td>0 Ω</td>
<td>Source resistance</td>
</tr>
<tr>
<td>$T_{NOM}$</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>$V_{TO}$</td>
<td>0 V</td>
<td>Zero-bias threshold voltage</td>
</tr>
<tr>
<td>$W$</td>
<td>50e-6 m</td>
<td>Gate width</td>
</tr>
<tr>
<td>$\Gamma$ (GAMMA)</td>
<td>0 $\sqrt{0.5}$</td>
<td>Bulk threshold parameter</td>
</tr>
<tr>
<td>$\Phi$ (PHI)</td>
<td>0.5 V</td>
<td>Surface potential</td>
</tr>
<tr>
<td>$\Lambda$ (LAMBDA)</td>
<td>0 1/V</td>
<td>Channel-length modulation</td>
</tr>
</tbody>
</table>

**Diode**

Figure 3-3 illustrates equivalent circuit for the diode.
Figure 3-3: A circuit for the diode.

The following equations are used to compute the relations between currents and voltages in the circuit.
where the following model parameters are required.

\[
i_d = i_{dhl} + i_{drec} + i_{db} + i_e
\]

\[
i_{dhl} = I_S \left( e^{\frac{v_d}{NVT} - 1} \right) \frac{1}{1 + I_S \left( e^{\frac{v_d}{NVT} - 1} \right)}
\]

\[
i_{drec} = I_{SR} \left( e^{\frac{v_d}{NVT} - 1} \right)
\]

\[
i_{db} = I_{BV} e^{\frac{v_d + BV}{NVT}}
\]

\[
C_j = C_{j0} \times \begin{cases} 
(1 - \frac{v_d}{V_T})^{-M} & v_d < FC V_T \\
(1 - FC)^{-1 - M} \left( 1 - FC(1 + M) + M \frac{v_d}{V_T} \right) & v_d \geq FC V_T 
\end{cases}
\]

\[
V_T = \frac{k_B T_{NOM}}{q}
\]

### TABLE 3-3: DIODE TRANSISTOR MODEL PARAMETERS

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>(B_V)</td>
<td>Inf (V)</td>
<td>Reverse breakdown voltage</td>
</tr>
<tr>
<td>(C_{j0})</td>
<td>0 F</td>
<td>Zero-bias junction capacitance</td>
</tr>
<tr>
<td>(F_C)</td>
<td>0.5</td>
<td>Forward-bias capacitance coefficient</td>
</tr>
<tr>
<td>(I_{BV})</td>
<td>1e-09 A</td>
<td>Current at breakdown voltage</td>
</tr>
<tr>
<td>(I_{KF})</td>
<td>Inf (A)</td>
<td>Corner for high-current roll-off</td>
</tr>
<tr>
<td>(I_S)</td>
<td>1e-13 A</td>
<td>Saturation current</td>
</tr>
<tr>
<td>(M)</td>
<td>0.5</td>
<td>Grading coefficient</td>
</tr>
<tr>
<td>(N)</td>
<td>1</td>
<td>Ideality factor</td>
</tr>
<tr>
<td>(N_{BV})</td>
<td>1</td>
<td>Breakdown ideality factor</td>
</tr>
<tr>
<td>(N_R)</td>
<td>2</td>
<td>Recombination ideality factor</td>
</tr>
<tr>
<td>(R_S)</td>
<td>0 Ω</td>
<td>Series resistance</td>
</tr>
<tr>
<td>(T_{NOM})</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>(V_J)</td>
<td>1.0 V</td>
<td>Junction potential</td>
</tr>
</tbody>
</table>
Reference for the Electrical Circuit Interface

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

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 non-circuit physics interface and return a current from the 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, 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 non-circuit physics interface feature, which then announces (that is, includes) the coupling to the Electrical Circuit interface. Its voltage or current is then included to make it visible to the connecting circuit feature.
- A voltage or current that has been announced (that is, included) is selected in a feature node’s settings window.

These circuit connections are supported in Terminals CoilsandLumpedPorts.

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 non-circuit physics interface.
- Define your own voltage or current measurement in the non-circuit 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 (compl.currents)**. The variable name is shown on the **State** settings window.

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.

**Solving**

Some modeling errors lead to the error message *The DAE is structurally inconsistent*, being displayed when solving. This 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 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 1D Plot Group node). The interface defines a Node voltage variable for each electrical node in the circuit, with name cir.v_<name>, where cir is the physics interface identifier and <name> is the node name. For each two pin component, the interface also defines variables containing the voltage across it and the current flowing through it.

In the COMSOL Multiphysics Reference Manual:
- Derived Values and Tables and Global Evaluation
- Plot Groups and Plots and Global
Spice Import

The circuit definition in COMSOL Multiphysics adheres to the SPICE format developed at the University of California, Berkeley (Ref. 1). 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>
<thead>
<tr>
<th>STATEMENT</th>
<th>DEVICE MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>Resistor</td>
</tr>
<tr>
<td>C</td>
<td>Capacitor</td>
</tr>
<tr>
<td>L</td>
<td>Inductor</td>
</tr>
<tr>
<td>V</td>
<td>Voltage Source</td>
</tr>
<tr>
<td>I</td>
<td>Current Source</td>
</tr>
<tr>
<td>E</td>
<td>Voltage-Controlled Voltage Source</td>
</tr>
<tr>
<td>F</td>
<td>Current-Controlled Current Source</td>
</tr>
<tr>
<td>G</td>
<td>Voltage-Controlled Current Source</td>
</tr>
<tr>
<td>H</td>
<td>Current-Controlled Voltage Source</td>
</tr>
<tr>
<td>D</td>
<td>Diode</td>
</tr>
<tr>
<td>Q</td>
<td>NPN BJT</td>
</tr>
<tr>
<td>M</td>
<td>n-Channel MOSFET</td>
</tr>
<tr>
<td>X</td>
<td>Subcircuit Instance</td>
</tr>
</tbody>
</table>

The 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.
Reference for SPICE Import

1. http://bwrc.eecs.berkeley.edu/Classes/IcBook/SPICE/
This chapter has information about the enhanced Laminar Flow interface available under the **Fluid Flow > Single-Phase Flow** branch ( |= ) when adding a physics interface.

In this chapter:

- The Single-Phase Flow, Laminar Flow Interface
- Theory for the Single-Phase Flow Laminar Interface
The Single-Phase Flow, Laminar Flow Interface

The Laminar Flow Interface

The Laminar Flow (spf) interface ( ), found under the Single-Phase Flow branch ( ), when adding a physics interface, is used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. A flow will remain laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence. This critical Reynolds number depends on the model, but a classical example is pipe flow where the critical Reynolds number is known to be approximately 2000.

The physics interface supports incompressible flows and compressible flows at low Mach numbers (typically less than 0.3). It also supports non-Newtonian fluids.

The equations solved by the Laminar Flow interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Laminar Flow interface can be used for stationary and time-dependent analyses. Note that for higher Reynolds numbers, a flow becomes inherently time dependent and three-dimensional, and time-dependent studies have to be used.

When this physics interface is added, the following default nodes are also added in the Model Builder—Fluid Properties, Wall (the default boundary condition is No slip), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click Laminar Flow to select physics from the context menu.

INTERFACE IDENTIFIER

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

The default identifier (for the first physics interface in the component) is spf.
PHYSICAL MODEL
By default the physics interface uses the Compressible flow (Ma<0.3) formulation of the Navier-Stokes equations. Select Incompressible flow to use the incompressible (constant density) formulation.

DEPENDENT VARIABLES
The following dependent variables (fields) are defined for this physics interface—the Velocity field \( \mathbf{u} \) (SI unit: m/s) and its components, and the Pressure \( p \) (SI unit: Pa).

If required, edit the field, component, and dependent variable names. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type, or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

CONSISTENT STABILIZATION
To display this section, click the Show button ( ) and select Stabilization.

The consistent stabilization methods applicable to the Navier-Stokes equations are Streamline diffusion and Crosswind diffusion. These check boxes are selected by default. If required, click to clear one or both of the Streamline diffusion and Crosswind diffusion check boxes. Observe that using P1+P1 elements requires Streamline diffusion to be active. If you deactivate Streamline diffusion, make sure that your model uses P2+P1 elements or higher.

INCONSISTENT STABILIZATION
To display this section, click the Show button ( ) and select Stabilization. By default, the Isotropic diffusion check box is not selected for the Navier-Stokes equations. Click to select as required.

ADVANCED SETTINGS
To display this section, click the Show button ( ) and select Advanced Physics Options. Normally these settings do not need to be changed.

Select the Use pseudo time stepping for stationary equation form check box to add pseudo time derivatives to the equation when the Stationary equation form is used. When selected, also choose a CFL number expression—Automatic (the default) or Manual. Automatic sets the local CFL number (from the Courant–Friedrichs–Lewy...
condition) to the built-in variable CFL_CMP which in turn triggers a PID regulator for the CFL number. If Manual is selected, enter a Local CFL number CFL_loc (dimensionless).

**DISCRETIZATION**

To display this section, click the Show button ( ) and select Discretization. It controls the discretization (the element types used in the finite element formulation). From the Discretization of fluids list select the element order for the velocity components and the pressure: P1+P1 (the default), P2+P1, or P3+P2.

- **P1+P1** (the default) means linear elements for both the velocity components and the pressure field. This is the default element order for the Laminar Flow interface. Linear elements are computationally cheaper than higher-order elements and are also less prone to introducing spurious oscillations, thereby improving the numerical robustness. P1+P1 elements require streamline diffusion to be a numerically valid discretization. Make sure that Streamline Diffusion in the Consistent Stabilization section is selected when using P1+P1 elements.

- **P2+P1** means second-order elements for the velocity components and linear elements for the pressure field.

- **P3+P2** means third-order elements for the velocity components and second-order elements for the pressure field. This can add additional accuracy but it also adds additional degrees of freedom compared to P2+P1 elements.

Specify the Value type when using splitting of complex variables—Real (the default) or Complex for each of the variables in the table.
Flow Past a Cylinder: model library path
COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow

For 2D axisymmetric models, COMSOL Multiphysics takes the axial symmetry boundaries (at \( r = 0 \)) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

### Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

The following nodes are for all physics interfaces found under the [Fluid Flow\>Single-Phase Flow](#) branch (�建) when adding a physics interface. Other physics interfaces also share many of these domain, boundary, pair, and point 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).

<table>
<thead>
<tr>
<th>Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>In general, to add a node, go to the <strong>Physics</strong> toolbar, no matter what operating system you are using.</td>
</tr>
</tbody>
</table>

- No Viscous Stress
- Flow Continuity
- Fluid Properties
- Initial Values
- Inlet
- Line Mass Source* 
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source* 
- Pressure Point Constraint
- Symmetry
- Vacuum Pump
- Volume Force
- Wall

* A feature that might require an additional license
For 2D axisymmetric models, COMSOL Multiphysics takes the axial symmetry boundaries (at \( r = 0 \)) into account and adds an Axial Symmetry node that is valid on the axial symmetry boundaries only.

**Fluid Properties**

The Fluid Properties node adds the momentum equations solved by the physics interface, except for volume forces which are added by the Volume Force feature. The node also provides an interface for defining the material properties of the fluid.

**Model Inputs**

Edit input variables to the fluid-flow equations if required. For fluid flow, these are typically introduced when a material requiring inputs has been selected.

**Absolute Pressure**

This input appears when a material requires the absolute pressure as model input. The absolute pressure input controls the pressure used to evaluate material properties, but it also relates to the value of the pressure field. There are usually two ways to calculate the pressure when describing fluid flow. Either solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

Which option to choose usually depends on the system and the equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, reduces the stability and convergence properties of the solver. In other cases, you can solve for the absolute pressure, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients.

The default Absolute pressure \( p_A \) (SI unit: Pa) is \( p + p_{\text{ref}} \) where \( p \) defaults to the pressure variable from the Navier-Stokes or RANS equations and \( p_{\text{ref}} \) to 1 [atm] (1 atmosphere = 101,325 Pa). The default setting is to solve for a gauge pressure.

If the pressure field instead is an absolute pressure field, clear the Reference pressure check box.
To model an incompressible fluid, set **Absolute pressure** $p_A$ to **User defined** and enter the desired pressure level in the edit field. The default value is $1\text{ atm}$.

---

This makes it possible to use a system-based (gauge) pressure as the pressure variable while automatically including the reference pressure in places where it is required, such as for gas flow governed by the gas law. While this check box maintains control over the pressure variable and instances when absolute pressure is required within this specific physics interface, it can not do so within other physics interfaces that it is coupled to. In such models, check the coupling between any physics interfaces using the same variable.

---

**FLUID PROPERTIES**

The default **Density** $\rho$ (SI unit: $\text{kg/m}^3$) uses the value **From material**. Select **User defined** to enter a different value or expression.

The default **Dynamic viscosity** $\mu$ (SI unit: $\text{Pa} \cdot \text{s}$) uses the value **From material** and describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities. Select **User defined** to define a different value or expression.

---

Using the built-in variable for the shear rate magnitude, $\text{spf} \cdot \text{sr}$, makes it possible to define arbitrary expressions of the dynamic viscosity as a function of the shear rate.

---

**Volume Force**

The **Volume Force** node specifies the volume force $\mathbf{F}$ on the right-hand side of the momentum equation. Use it, for example, to incorporate the effects of gravity in a model.

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

If several volume force nodes are added to the same domain, then the sum of all contributions are added to the momentum equations.
VOLUME FORCE
Enter the components of the Volume force $\mathbf{F}$ (SI unit: N/m$^3$). The defaults for all components are 0 N/m$^3$.

Initial Values
The Initial Values node adds initial values for the velocity field and the pressure that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

COORDINATE SYSTEM SELECTION
The Global coordinate system is selected by default. The Coordinate system list contains any additional coordinate systems that the component includes.

INITIAL VALUES
Enter values or expressions for the initial value of the Velocity field $\mathbf{u}$ (SI unit: m/s) and the Pressure $p$ (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Wall
The Wall node includes a set of boundary conditions describing the fluid-flow condition at a wall.
- No Slip (the default)
- Slip
- Sliding Wall
- Moving Wall
- Leaking Wall
- Slip Velocity

BOUNDARY SELECTION
For a default node, the setting inherits the selection from the parent node, and can not be edited; that is, the selection is automatically made and is the same as for the physics
interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific boundaries or select All boundaries as required.

**BOUNDARY CONDITION**

Select a Boundary condition for the wall.

**No Slip**

No slip is the default boundary condition for a stationary solid wall for laminar flow. The condition prescribes \( u = 0 \), that is, the fluid at the wall is not moving.

**Slip**

The Slip option prescribes a no-penetration condition, \( u \cdot n = 0 \). It hence implicitly assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

**Sliding Wall**

The Sliding wall boundary condition is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

---

For 3D models, enter the components of the **Velocity of the sliding wall** \( u_w \) (SI unit: m/s). If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.

---

For 2D models, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, the sliding wall boundary condition has slightly different definitions in the different space dimensions. Enter the components of the **Velocity of the tangentially moving wall** \( U_w \) (SI unit: m/s).
**Moving Wall**

If the wall moves, so must the adjacent fluid. Hence, this boundary condition prescribes $u = \mathbf{u}_w$. Enter the components of the Velocity of moving wall $\mathbf{u}_w$ (SI unit: m/s).

Specifying this boundary condition does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

**Leaking Wall**

Use this boundary condition to simulate a wall where fluid is leaking into or leaving through a perforated wall $u = u_l$. Enter the components of the Fluid velocity $u_l$ (SI unit: m/s).

**Slip Velocity**

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a Slip velocity at the boundary. Two phenomena account for this velocity: the noncontinuum effects and flow induced by a thermal gradient along the boundary. Enter the Velocity of moving wall: $\mathbf{u}_w$ (SI unit: m/s). The defaults are 0 m/s.

If the Use viscous slip check box is selected, the default Slip length $L_s$ (SI unit: m) is User defined. Enter another value or expression if the default of $1 \times 10^{-7}$ m is not applicable.

If Maxwell’s Model is selected, enter values or expressions for the Tangential momentum accommodation coefficient $a_v$ and the Mean free path $\lambda$ (SI unit: m).

**Tangential accommodation coefficients** are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

If the Use thermal creep check box is selected, it activates the thermal creep component of the boundary condition. By default, the fluid Temperature $T$ (SI unit: K) is 293.15 K and the default Thermal slip coefficient $\sigma_T$ (dimensionless) is 0.75.

**Thermal slip coefficients** are typically between 0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.
CONTRAINT SETTINGS
To display this section, click the Show button ( ) and select Advanced Physics Options.

For the No Slip, Moving Wall, and Leaking Wall boundary conditions, select an option from the Apply reaction terms on: list—All physics (symmetric) or Individual dependent variables. The other types of wall boundary conditions with constraints use Individual dependent variables constraints only.

Select the Use weak constraints check box (not available for the Sliding Wall condition) to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

Inlet
The Inlet node includes a set of boundary conditions describing the fluid-flow conditions at an inlet. The Velocity boundary condition is the default.

In many cases the Inlet boundary conditions are available, some of them slightly modified, for the Outlet type as well. For certain conditions there is nothing in the mathematical formulations to prevent the fluid from leaving the domain through boundaries where the Inlet type is specified.

Prescribing Inlet and Outlet Conditions
Pressure, No Viscous Stress Boundary Condition
Normal Stress Boundary Condition
BOUNDARY CONDITION
Select a Boundary condition for the inlet—Velocity (the default), Pressure, No Viscous Stress, Laminar Inflow, Mass Flow, or Normal Stress.

After selecting a Boundary Condition from the list, a section with the same name displays underneath. For example, if Velocity is selected, a Velocity section displays where further settings are defined for the velocity.

VELOCITY
The Velocity boundary condition is available for the Inlet and Outlet boundary nodes.

- Select Normal inflow velocity (the default) to specify a normal inflow velocity magnitude \( u = -n U_0 \) where \( n \) is the boundary normal pointing out of the domain. Enter the velocity magnitude \( U_0 \) (SI unit: m/s). The default is 0 m/s.
- If Velocity field is selected, it sets the velocity equal to a given velocity vector \( \mathbf{u}_0 \) when \( \mathbf{u} = \mathbf{u}_0 \). Enter the components of \( \mathbf{u}_0 \) (SI unit: m/s). The defaults are 0 m/s.

PRESSURE, NO VISCOUS STRESS
The Pressure, no viscous stress boundary condition is available for the Inlet boundary node. It specifies vanishing viscous stress along with a Dirichlet condition on the pressure. Enter the Pressure \( p_0 \) (SI unit: Pa) at the boundary. The default is 0 Pa.

Depending on the pressure field in the rest of the domain, an inlet boundary with this condition can become an outlet boundary.

NORMAL STRESS
The Normal stress boundary condition is available for the Inlet, Outlet (via the Pressure condition), Open Boundary, and No Viscous Stress nodes. Enter the magnitude of Normal stress \( f_0 \) (SI unit: N/m²). This implicitly imposes \( p \approx f_0 \). The default is 0 N/m².

LAMINAR INFLOW
The Laminar inflow boundary condition is available for the Inlet node.
Select a flow quantity for the inlet—**Average velocity** (the default), **Flow rate**, or **Entrance pressure**.

- When **Average velocity** is selected, enter an **Average velocity** $U_{av}$ (SI unit: m/s). The default is 0 m/s.
- If **Flow rate** is selected, enter the **Flow rate** $V_0$ (SI unit: m$^3$/s). The default is 0 m$^3$/s.
- If **Entrance pressure** is selected, enter the **Entrance pressure** $p_{ent}$ (SI unit: Pa) at the entrance of the fictitious channel outside of the model. The default is 0 Pa.

Then for any selection, specify the entrance length and constraints:

- Enter the **Entrance length** $L_{ent}$ (SI unit: m) to define the length of the inlet channel outside the model domain.

---

The **Entrance length** value must be large enough so that the flow can reach a laminar profile. For a laminar flow, $L_{ent}$ should be significantly greater than $0.06\Re D$, where $\Re$ is the Reynolds number and $D$ is the inlet length scale (this formula is exact if $D$ is the diameter of a cylindrical pipe and approximate for other geometries).

- Select the **Constrain outer edges to zero** (for 3D models) or **Constrain endpoints to zero** (for 2D and 2D axisymmetric models) check box to force the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the model. For example, if one end of a boundary with a laminar inflow condition connects to a slip boundary condition, then the laminar profile has a maximum at that end.

**MASS FLOW**

The **Mass flow** boundary condition is available for the **Inlet** node. However, depending on the sign of the specified mass flow or flux, an inlet boundary with this condition can become an outlet boundary.

Select a **Mass flow type**—**Mass flow rate** (the default), **Pointwise mass flux**, **Standard flow rate**, or **Standard flow rate (SCCM)**.

**Mass Flow Rate**

The **Mass flow rate** sets the integrated mass flow across the entire boundary to a specific value. The mass flow is assumed to be parallel to the boundary normal, so the tangential velocity is set to zero.
Enter the **Normal mass flow rate** \( m \) (SI unit: kg/s). The default value is \( 10^{-5} \) kg/s.

For 2D models, enter a **Channel thickness** \( d_{bc} \) (SI unit: m). The default value is 1 m.

The **Channel thickness** is used only in defining the area across which the mass flow occurs—it is not a setting applied to the whole model. Line or surface integrals of the mass flux over the boundary evaluated during post-processing or using when integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

**Pointwise Mass Flux**

The **Pointwise mass flux** sets the mass flux parallel to the boundary normal. The flux perpendicular to the normal is set to zero. The mass flux is a model input, which means that COMSOL Multiphysics can take its value from another physics interface if applicable. If **User defined** is selected from the **Mass flux** list, enter a value for \( M_f \) (SI unit: kg/(m\(^2\)·s)). The default value is 0 kg/(m\(^2\)·s).

**Standard Flow Rate**

The **Standard flow rate** sets a standard volumetric flow rate, according to the SEMI standard E12-0303. The flow rate is specified as the volumetric flow rate that would occur for the same number of moles per second, if the gas density were a standard value (the molar mass over a fixed standard volume). The flow occurs across the whole boundary in the direction of the boundary normal and is computed by a surface (3D) or line (2D) integral. The tangential flow velocity is set to zero.

The standard density can be defined directly, or by specifying a standard pressure and temperature, in which case the ideal gas law is assumed. Select an option from the **Standard flow rate defined by** list—**Standard density** (the default) or **Standard pressure and temperature**.

For either option enter the following values:

- **Standard flow rate** \( Q_{sv} \) (SI unit: m\(^3\)/s) to specify the standard volumetric flow rate through the boundary. The default value is \( 10^{-6} \) m\(^3\)/s.
- **Mean molar mass** \( M_m \) (SI unit: kg/mol). This can be selected as a model input from another physics interface or, if **User defined** is selected, you can either keep the default (0.032 kg/mol) or enter another value or expression.
If **Standard density** is selected also enter the **Standard molar volume** $V_m$ (SI unit: m$^3$/mol). The default is 0.0224136 m$^3$/mol.

If **Standard pressure and temperature** is selected, also enter the **Standard pressure** $P_{st}$ (SI unit: Pa) (the default is 1 atm (101,325 Pa)) and the **Standard temperature** $T_{st}$ (SI unit: K). The default is 273.15 K (0 degrees Celsius).

---

**Standard Flow Rate (SCCM)**

The **Standard flow rate (SCCM)** boundary condition is equivalent to the **Standard flow rate** boundary condition, except that the flow rate is entered directly in SCCMs (standard cubic centimeters per minute) without a requirement to specify the units. Enter the **Number of SCCM units** $Q_{sccm}$ (dimensionless). The default is 100.

**CONTRAINT SETTINGS**

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**. Select the **Use weak constraints** check box to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

When **Velocity** or **Pressure, No Viscous Stress** are selected as the **Boundary condition**, and to **Apply reaction terms on** all dependent variables, select **All physics (symmetric)**. Or select **Individual dependent variables** to restrict the reaction terms as required.

---

**Outlet**

The **Outlet** node includes a set of boundary conditions describing fluid-flow conditions at an outlet. **Pressure** is the default. Other options are based on individual licenses. Selecting appropriate outlet conditions for the Navier-Stokes equations is not a trivial
Some of the formulations for the Outlet type are also available, possibly slightly modified, in other boundary types. For certain conditions there is nothing in the mathematical formulations to prevent the fluid from entering a domain through boundaries where the Outlet boundary type is specified.

**BOUNDARY CONDITION**

Select a Boundary condition for the outlet—Pressure (the default), Laminar Outflow, or Velocity.

The Velocity boundary condition is described for the Inlet node.

**Pressure**

The Pressure condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 N/m².

- Enter the Pressure \( p_0 \) (SI unit: Pa) at the boundary. The default is 0 Pa.
- Select the Normal flow check box to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The Suppress backflow check box is selected by default. This option adjusts the outlet pressure in order to prevent fluid from entering the domain through the boundary.

**Laminar Outflow**

This section displays when Laminar outflow is selected as the Boundary condition. Select a flow quantity to specify for the inlet:

- If Average velocity is selected, enter an Average velocity \( U_{av} \) (SI unit: m/s). The default is 0 m/s.
• If Flow rate is selected, enter the Flow rate $V_0$ (SI unit: m$^3$/s). The default is 0 m$^3$/s.
• If Exit pressure is selected, enter the Exit pressure $P_{\text{exit}}$ (SI unit: Pa) at the end of the fictitious channel following the outlet. The default is 0 Pa.

Then specify the Exit length and Constrain endpoints to zero parameters:
Enter the Exit length $L_{\text{exit}}$ (SI unit: m) to define the length of the fictitious channel outside the model domain.

The Exit length value must be large enough so that the flow can reach a laminar profile. For a laminar flow, $L_{\text{exit}}$ should be significantly greater than $0.06 \text{Re} D$, where $\text{Re}$ is the Reynolds number and $D$ is the outlet length scale (this formula is exact if $D$ is the diameter of a cylindrical pipe and approximate for other geometries).

Select the Constrain outer edges to zero (3D models) or Constrain endpoints to zero (2D models) check box to force the laminar profile to go to zero at the bounding points or edges of the inlet channel. Otherwise the velocity is defined by the boundary condition of the adjacent boundary in the model. For example, if one end of a boundary with a Laminar outflow condition connects to a Slip boundary condition, then the laminar profile has a maximum at that end.

CONSTRAINT SETTINGS
To display this section, click the Show button ( ) and select Advanced Physics Options. Select the Use weak constraints check box to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

When Velocity or Pressure is selected as the Boundary condition, and to Apply reaction terms on all dependent variables, select All physics (symmetric). Or select Individual dependent variables to restrict the reaction terms as required.

Symmetry

The Symmetry node adds a boundary condition that describes symmetry boundaries in a fluid-flow simulation. The boundary condition for symmetry boundaries prescribes no penetration and vanishing shear stresses. The boundary condition is a combination of a Dirichlet condition and a Neumann condition:

$$u \cdot n = 0, \quad (-p I + \mu \nabla u + (\nabla u)^T) \cdot n = 0$$
CHAPTER 4: THE FLUID FLOW BRANCH

for the compressible and incompressible formulations. The Dirichlet condition takes precedence over the Neumann condition, and the above equations are equivalent to the following equation for both the compressible and incompressible formulations:

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = 0 \]

BOUNDARY SELECTION

From the Selection list, choose the boundaries on which to apply the condition.

CONSTRAINT SETTINGS

To display this section, click the Show button ( ) and select Advanced Physics Options. Select the Use weak constraints check box to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

Open Boundary

The Open Boundary node adds boundary conditions describing boundaries in contact with large volumes of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

BOUNDARY CONDITIONS

Select a Boundary condition for the open boundaries—Normal Stress (the default) or Laminar Outflow. The Normal stress condition is described for the Inlet node.

No Viscous Stress

The No Viscous Stress condition specifies vanishing viscous stress on the outlet. This condition does not provide sufficient information to fully specify the flow at the outlet and must at least be combined with pressure constraints on adjacent points.

If No viscous stress is selected, it prescribes vanishing viscous stress:
The *Boundary Stress* node adds a boundary condition that represents a very general class of conditions also known as traction boundary conditions.

**Boundary Condition**

Select a *Boundary condition* for the boundary stress—*General stress* (the default), *Normal Stress* (described for the Inlet node), or *Normal stress, normal flow*.

**General Stress**

When *General stress* is selected, enter the components for the *Stress* \( \mathbf{F} \) (SI unit: \( \text{N/m}^2 \)). The total stress on the boundary is set equal to a given stress \( \mathbf{F} \):

\[
\left( -p \mathbf{I} + \left( \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\mathbf{u} \cdot \mathbf{I}) \right) \right) \mathbf{n} = \mathbf{F}
\]

\[
(-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = \mathbf{F}
\]

This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, combine this boundary condition with a point constraint on the pressure.

This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, combine this boundary condition with a point constraint on the pressure.

\[
\left( \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\mathbf{u} \cdot \mathbf{I}) \right) \mathbf{n} = 0
\]

using the compressible and the incompressible formulations.

\[
\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} = 0
\]
Normal Stress, Normal Flow

If Normal stress, normal flow is selected, enter the magnitude of the Normal stress \( f_0 \) (SI unit: N/m\(^2\)).

In addition to the stress condition set in the Normal Stress condition, the Normal stress, normal flow condition also prescribes that there must be no tangential velocities on the boundary:

\[
\left( -p \mathbf{I} + \left( \mu \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \right) \mathbf{n} = -f_0 \mathbf{n}, \quad \mathbf{t} \cdot \mathbf{u} = 0
\]

\[
\left( -p \mathbf{I} + \mu \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \mathbf{n} = -f_0 \mathbf{n}, \quad \mathbf{t} \cdot \mathbf{u} = 0
\]

using the compressible and the incompressible formulations.

This boundary condition also implicitly sets a constraint on the pressure that for 2D flows is

\[
p = 2 \mu \frac{\partial u_n}{\partial n} + f_0
\]

(4-2)

If \( \partial u_n / \partial n \) is small, Equation 4-2 states that \( p \approx f_0 \).

Constraint Settings

To display this section, click the Show button ( ) and select Advanced Physics Options. Select the Use weak constraints check box to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

If Normal Stress, Normal Flow is selected as the Boundary condition, then to Apply reaction terms on all dependent variables, select All physics (symmetric). Or select Individual dependent variables to restrict the reaction terms as required.

Vacuum Pump

The Vacuum Pump node models the effective outlet pressure created by a vacuum pump device that is attached to the outlet.

Parameters

Select a Static pressure curve to define a lumped curve—Linear (the default), Static pressure curve data, or User defined.
Linear
If Linear is selected, enter values or expressions for the Static pressure at no flow \( p_{nf} \) (SI unit: Pa) and the Free delivery flow rate \( V_{0,fd} \) (SI unit: m\(^3\)/s). The defaults are 100 Pa and 0.01 m\(^3\)/s, respectively.

The static pressure curve is equal to the static pressure at no flow rate when \( V_0 < 0 \) and equal to 0 when the flow rate is larger than the free delivery flow rate.

Static Pressure Curve Data
Select Static pressure curve data to enter or load data under the Static Pressure Curve Data section that displays. The interpolation between points given in the Static Pressure Curve Data table is defined using the Interpolation function type list in the Static Pressure Curve Interpolation section.

User Defined
Select User defined to enter different values or expressions. The flow rate across the selection where this boundary condition is applied is defined by \( \text{phys}_id.V0 \) where \( \text{phys}_id \) is the physics interface identifier (for example, \( \text{phys}_id \) is spf by default for this physics interface). In order to avoid unexpected behavior, the function used for the fan curve is the maximum of the user-defined function and 0.

Static Pressure Curve Data
This section is available when Static pressure curve data is selected as the Static pressure curve. In the table, enter values or expressions for the Flow rate and Static pressure curve (or click the Load from file button ( ) under the table to import a text file). Select the Flow rate (the default SI unit is m\(^3\)/s) and Static pressure curve (the default SI unit is Pa).

Static Pressure Curve Interpolation
This section is available when Static pressure curve data is selected as the Static pressure curve. Select the Interpolation function type—Linear (the default), Piecewise cubic, or Cubic spline.

The extrapolation method always returns a constant value. In order to avoid problems with an undefined function, the function used for the boundary condition is the maximum of the interpolated function and 0.
Periodic Flow Condition

The Periodic Flow Condition splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

Vacuum Pump Boundary Condition

If the boundaries are curved, it is recommended to only include two boundaries.

No input is required when Compressible flow (Ma<0.3) is selected as the Compressibility option under the Physical Model section for the physics interface. Typically when a periodic boundary condition is used with a compressible flow the pressure is the same at both boundaries and the flow is driven by a volume force.

Pressure Difference

This section is available when Incompressible flow is selected as the Compressibility option under the Physical Model section for the physics interface.

Enter a value or expression for the pressure difference, $p_{\text{src}} - p_{\text{dst}}$ (SI unit: Pa). This pressure difference can, for example, drive the fully developed flow in a channel. The default is 0 Pa.

To set up a periodic boundary condition select both boundaries in the Periodic Flow Condition node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, add a Destination Selection node to the Periodic Flow Condition node. All destination sides must be connected.
**CONSTRAINT SETTINGS**

To display this section, click the Show button ( ) and select Advanced Physics Options. Select the Use weak constraints check box to use weak constraints and create dependent variables for the corresponding Lagrange multipliers.

---

**Flow Continuity**

The Flow Continuity node is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The Wall feature can be overridden by any other boundary condition that applies to exterior boundaries. Right-click the Flow Continuity node to add additional subnodes.

---

**Point Mass Source**

The Point Mass Source feature models mass flow originating from an infinitely small domain centered around a point.

---

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, the Point Mass Source node is available as two nodes, one for the fluid flow (Fluid Point Source) and one for the species (Species Point Source).
CHAPTER 4: THE FLUID FLOW BRANCH

POINT SELECTION

The Point Mass Source feature is available in 3D where it can be added to any point and in 2D axisymmetry where it can be added to points on the symmetry axis.

SOURCE STRENGTH

Enter the Mass flux, $q_p$, for the source (SI unit: kg/s). A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

Point sources located on a boundary or on an edge affects the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.


Line Mass Source

The Line Mass Source feature models mass flow originating from a tube region with infinitely small radius.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, the Line Mass Source node is available as two nodes, one for the fluid flow (Fluid Line Source) and one for the species (Species Line Source).
SELECTION
The Line Mass Source feature is available for all dimensions, but the applicable selection differs between the dimensions.

<table>
<thead>
<tr>
<th>MODEL DIMENSION</th>
<th>APPLICABLE GEOMETRICAL ENTITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>Points</td>
</tr>
<tr>
<td>2D Axisymmetry</td>
<td>Points not on the symmetry axis and the symmetry axis</td>
</tr>
<tr>
<td>3D</td>
<td>Edges</td>
</tr>
</tbody>
</table>

SOURCE STRENGTH
Enter the Mass flux, \( \dot{q}_1 \), for the source (SI unit: \( \text{kg}/(\text{s} \cdot \text{m}) \)). A positive value results in mass being ejected from the line into the computational domain and a negative value means that mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This, for example, has the effect that the physical strength of a line source located in a symmetry plane is twice the given strength.

Pressure Point Constraint
The Pressure Point Constraint node adds a pressure constraint at a point. If it is not possible to specify the pressure level using a boundary condition, the pressure level must be set in some other way, for example, by specifying a fixed pressure at a point.

PRESSURE CONSTRAINT
Enter a point constraint for the Pressure \( p_0 \) (SI unit: Pa). The default is 0 Pa.
CONSTRAINT SETTINGS
To display this section, click the Show button ( ) and select Advanced Physics Options. To Apply reaction terms on all dependent variables, select All physics (symmetric). Or select Individual dependent variables to restrict the reaction terms as required. Select the Use weak constraints check box to replace the standard constraints with a weak implementation.
Theory for the Single-Phase Flow Laminar Interface

The Single-Phase Flow, Laminar Flow theory is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- The Boussinesq Approximation
- Theory for the Wall Boundary Condition
- Prescribing Inlet and Outlet Conditions
- Laminar Inflow
- Laminar Outflow
- Mass Flow
- No Viscous Stress
- Pressure, No Viscous Stress Boundary Condition
- Normal Stress Boundary Condition
- Vacuum Pump Boundary Condition
- Mass Sources for Fluid Flow
- Numerical Stability—Stabilization Techniques for Fluid Flow
- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Discontinuous Galerkin Formulation
- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces

The theory about most boundary conditions is found in Ref. 2.
General Single-Phase Flow Theory

The single-phase fluid-flow interfaces are based on the Navier-Stokes equations, which in their most general form read

\begin{align}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \quad (4-3) \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} &= \nabla \cdot [-p \mathbf{I} + \mathbf{\tau}] + \mathbf{F} \quad (4-4) \\
\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T\right) &= - (\nabla \cdot \mathbf{q}) + \mathbf{S} : \frac{T}{\rho} \frac{\partial p}{\partial T} \left[\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla)p\right] + Q \quad (4-5)
\end{align}

where

- \( \rho \) is the density (SI unit: kg/m\(^3\))
- \( \mathbf{u} \) is the velocity vector (SI unit: m/s)
- \( p \) is pressure (SI unit: Pa)
- \( \mathbf{\tau} \) is the viscous stress tensor (SI unit: Pa)
- \( \mathbf{F} \) is the volume force vector (SI unit: N/m\(^3\))
- \( C_p \) is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- \( T \) is the absolute temperature (SI unit: K)
- \( \mathbf{q} \) is the heat flux vector (SI unit: W/m\(^2\))
- \( Q \) contains the heat sources (SI unit: W/m\(^3\))
- \( \mathbf{S} \) is the strain-rate tensor:

\[ \mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \]

The operation “:” denotes a contraction between tensors defined by

\[ \mathbf{a} : \mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \quad (4-6) \]

This is sometimes referred to as the double dot product.

**Equation 4-3** is the continuity equation and represents conservation of mass.
**Equation 4-4** is a vector equation which represents conservation of momentum.
**Equation 4-5** describes the conservation of energy, formulated in terms of...
temperature. This is an intuitive formulation that facilitates boundary condition specifications.

To close the equation system, Equation 4-3 through Equation 4-5, constitutive relations are needed. For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

\[
\tau = 2\mu \mathbf{S} - \frac{2}{3}\mu (\nabla \cdot \mathbf{u}) \mathbf{I} \tag{4-7}
\]

The dynamic viscosity, \( \mu \) (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions.

Other commonly used constitutive relations are Fourier’s law of heat conduction and the ideal gas law.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

Many applications describe isothermal flows for which Equation 4-5 is decoupled from Equation 4-3 and Equation 4-4.

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 4-3 and Equation 4-4 requires \( \partial / \partial \phi \) to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is however that \( u_\phi = 0 \). In such cases, the \( \phi \)-equation can be removed from Equation 4-4. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the \( \phi \)-equation. The default 2D axisymmetric formulation of Equation 4-3 and Equation 4-4 therefore assumes that...
Compressible Flow

The Navier-Stokes equations solved by default in all Single-Phase Flow interfaces apply the compressible formulation of the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$  \hspace{1cm} (4-8)

and the momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left( \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$ \hspace{1cm} (4-9)

These equations are applicable for incompressible as well as compressible flow with density variations.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, $Ma$, defined by

$$Ma = \frac{|\mathbf{u}|}{a}$$

where $a$ is the speed of sound. A flow is formally incompressible when $Ma = 0$. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier-Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 4-9, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 4-8, is hyperbolic for both steady and unsteady flow. The combined system of equations is thus hybrid parabolic-hyperbolic for unsteady flow and hybrid elliptic-hyperbolic for steady flow. An exception occurs when the viscous term in Equation 4-9 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain.
For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well posed system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with Mach number larger than or equal to one.

The practical Mach number limit is lower than one, however. The main reason is that numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier-Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization in the Single-Phase Flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at $Ma = 0.3$. For this reason the compressible formulation is referred to as compressible flow ($Ma < 0.3$) in COMSOL Multiphysics.

Incompressible Flow

When the temperature variations in a flow are small, a single-phase fluid can often be assumed incompressible; that is, $\rho$ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant $\rho$, Equation 4-8 reduces to

$$ \rho \nabla \cdot \mathbf{u} = 0 $$ (4-10)

and Equation 4-9 becomes

$$ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-\rho I + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} $$ (4-11)

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

$$ Re = \frac{\rho U L}{\mu} $$
where \( U \) denotes a velocity scale, and \( L \) denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

Observe that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The \textbf{Fluid Flow} interfaces automatically calculate the local cell Reynolds number \( \text{Re}^c = \rho |u| h / (2 \mu) \) using the element length \( h \) for \( L \) and the magnitude of the velocity vector \( u \) for the velocity scale \( U \). This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as \( \text{Re}^c \) grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: \texttt{spf.cellRe}).

\textit{The Boussinesq Approximation}

The Boussinesq approximation is a way to treat certain simple cases of buoyant flows without having to use a compressible formulation of the Navier-Stokes equations.

The Boussinesq approximation assumes that variations in density have no effect on the flow field except that they give rise to buoyancy forces. The density is assigned a reference value, \( \rho_0 \), everywhere except in the body force term, which is set to

\begin{equation}
\mathbf{F} = (\rho_0 + \Delta \rho) \mathbf{g}
\end{equation}

where \( \mathbf{g} \) is the gravity vector. A further simplifications is often possible. Since \( \mathbf{g} \) can be written in terms of a potential, \( \Phi \), it is possible to write Equation 4-12 as:

\begin{equation}
\mathbf{F} = - \nabla (\rho_0 \Phi) + \Delta \rho \mathbf{g}
\end{equation}

The first part can be canceled out by splitting the true pressure, \( p \), into a hydrodynamic component, \( P \), and a hydrostatic component, \( -\rho_0 \Phi \). Equation 4-10 and Equation 4-11 are expressed in terms of the hydrodynamic pressure \( P = p + \rho_0 \Phi \):

\begin{equation}
\rho \nabla \cdot \mathbf{u} = 0
\end{equation}
To obtain the Boussinesq approximation in this form, enter the expression for $g\Delta\rho$ for the Volume Force feature.

In practice, the shift from $p$ to $P$ can be ignored except where the pressure appears in boundary conditions. The pressure that is specified at boundaries is the hydrodynamic pressure in this case. For example, on a vertical outflow or inflow boundary, the hydrodynamic pressure is typically a constant, while the true pressure is a function of the vertical coordinate.

The system that Equation 4-13 and Equation 4-14 form has its limitations. The main assumption is that the density fluctuations must be small; that is, $\Delta\rho/\rho_0 \ll 1$. There are also some more subtle constraints that, for example, make the Boussinesq approximation unsuitable for systems of very large dimensions. An excellent discussion of the Boussinesq approximation and its limitations appears in Chapter 14 of Ref. 10.

**Theory for the Wall Boundary Condition**

**SLIP**

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = 0$$

The no penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to:

$$\rho_0 \frac{\partial \mathbf{u}}{\partial t} + (\rho_0 \mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla P + \nabla \cdot (\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + g\Delta\rho$$  (4-14)
\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n})\mathbf{n} = 0 \]

\[ \mathbf{K} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} \]

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

**SLIDING WALL**

The Sliding Wall boundary condition is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

<table>
<thead>
<tr>
<th>In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.</th>
</tr>
</thead>
</table>
| For 2D and 2D axisymmetric models, the velocity is given as a scalar \( \mathbf{U}_w \) and the condition prescribes
\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{u} \cdot \mathbf{t} = \mathbf{U}_w \]
where \( \mathbf{t} = (n_y, -n_x) \) for 2D and \( \mathbf{t} = (n_z, -n_r) \) for axial symmetry. |
| For 3D models, the velocity is set equal to a given vector \( \mathbf{u}_w \) projected onto the boundary plane:
\[ \mathbf{u} = \frac{\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w) \mathbf{n}}{||\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w) \mathbf{n}||} \mathbf{u}_w \]
The normalization makes \( \mathbf{u} \) have the same magnitude as \( \mathbf{u}_w \) even if \( \mathbf{u}_w \) is not exactly parallel to the wall. |

**SLIP VELOCITY**

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a slip velocity at the boundary. Two phenomena account for this velocity: violation of the continuum hypothesis for the viscosity and flow induced by a thermal gradient along the boundary.
The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary:

$$\Delta u = \frac{1}{\beta} \tau_{n,t}$$

For gaseous fluids, the coefficient $\beta$ is given by

$$\beta = \frac{\mu}{\left(\frac{2 - \alpha_v}{\alpha_v}\right) \lambda}$$

where $\mu$ is the fluid’s dynamic viscosity (SI unit: Pa·s), $\alpha_v$ represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and $\lambda$ is the molecules’ mean free path (SI unit: m). The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 15.

A simpler expression for $\beta$ is

$$\beta = \frac{\mu}{L_s}$$

where $L_s$, the slip length (SI unit: m), is a straight channel measure of the distance from the boundary to the virtual point outside the flow domain where the flow profile extrapolates to zero. This equation holds for both liquids and gases.

Thermal creep results from a temperature gradient along the boundary. The following equation relates the thermally-induced jump in tangential velocity to the tangential gradient of the natural logarithm of the temperature along the boundary:

$$\Delta u = \sigma_T \frac{\mu}{\rho} \nabla_{\!T} \log T$$

where $\sigma_T$ is the thermal slip coefficient (dimensionless) and $\rho$ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 15.

Combining the previous relationships results in the following equation:

$$u - u_{w,t} = \frac{L_s}{\mu} \tau_{n,t} + \sigma_T \frac{\mu}{\rho T} \nabla_{\!T} T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,t} = K - (n \cdot K)n$$
where the components of $K$ are the Lagrange multipliers that are used to implement the boundary condition. Similarly, the tangential temperature gradient results from the difference of the gradient and its normal projection:

$$\nabla_t T = \nabla T - (\mathbf{n} \cdot \nabla T) \mathbf{n}$$

**Use Viscous Slip**

When viscous slip is used, select Maxwell’s model to calculate $L_s$ using:

$$L_s = \left( \frac{2 - \alpha_v}{\alpha_v} \right) \lambda.$$ 

---

**Prescribing Inlet and Outlet Conditions**

The Navier-Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions.

---

**INLET CONDITIONS**

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure, in which case the normal velocity component is specified indirectly via the continuity equation. The pressure can be specified pointwise, which is a mathematically over-constraining but numerically robust formulation. This is achieved using the Pressure, No Viscous Stress condition. Alternatively, the pressure can be specified via a stress condition.
where $\frac{\partial u_n}{\partial n}$ is the normal derivative of the normal velocity component.

**Equation 4-15** is prescribed by the Normal stress condition. **Equation 4-15** is mathematically more stringent compared to specifying the pressure pointwise, can at the same time not guarantee that $p$ obtains the desired value. In practice, $p$ will however be close to $F_n$, except for low Reynolds number flows where viscous effects are the only effects that balance the pressure.

**OUTLET CONDITIONS**

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\frac{\partial u_t}{\partial n} = 0$$

where $\frac{\partial u_t}{\partial n}$ is the normal derivative of the tangential velocity field. It is also possible to prescribe $u_t$ to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

The elliptic character of the Navier-Stokes equations mathematically permit specifying a complete velocity field at an outlet. This can however be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it at each point is consistent with the interior solution. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

**ALTERNATIVE FORMULATIONS**

COMSOL provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they often prescribe a velocity or a pressure, but calculate the prescribed values using for example ODEs.

**Laminar Inflow**

In order to prescribe a fully developed inlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation
shown in Figure 4-1: a fictitious domain of length $L_{entr}$ is assumed to be attached to the inlet of the computational domain. The domain is an extrusion of the inlet boundary, which means that laminar inflow requires the inlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is fully developed laminar flow. The “wall” boundary conditions for the fictitious domain is inherited from the real domain, $\Omega$, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious “walls” are no-slip walls.

![Diagram](image)

Figure 4-1: An example of the physical situation simulated when using the Laminar inflow boundary condition. $\Omega$ is the actual computational domain while the dashed domain is a fictitious domain.

If an average inlet velocity or inlet volume flow is specified instead of the pressure, COMSOL Multiphysics adds an ODE that calculates a pressure, $p_{entr}$, such that the desired inlet velocity or volume flow is obtained.

**Laminar Outflow**

In order to prescribe an outlet velocity profile, this boundary condition adds a weak form contribution and constraints corresponding to unidirectional flow perpendicular to the boundary. The applied condition corresponds to the situation shown in Figure 4-2: assume that a fictitious domain of length $L_{exit}$ is attached to the outlet of the computational domain. The domain is an extrusion of the outlet boundary, which means that laminar outflow requires the outlet to be flat. The boundary condition uses the assumption that the flow in this fictitious domain is fully developed laminar flow. The “wall” boundary conditions for the fictitious domain is inherited from the real
domain, $\Omega$, unless the option to constrain outer edges or endpoints to zero is selected in which case the fictitious “walls” are no-slip walls.

![Figure 4-2: An example of the physical situation simulated when using the Laminar outflow boundary condition. $\Omega$ is the actual computational domain while the dashed domain is a fictitious domain.](image)

If the average outlet velocity or outlet volume flow is specified instead of the pressure, the software adds an ODE that calculates $p_{\text{exit}}$ such that the desired outlet velocity or volume flow is obtained.

**Mass Flow**

The **Mass Flow** boundary condition constrains the mass flowing into the domain across an inlet boundary. The mass flow can be specified in a number of ways.

**POINTWISE MASS FLUX**

The pointwise mass flux sets the velocity at the boundary to:

$$u = \frac{m_f}{p} n$$

where $m_f$ is the normal mass flux and $p$ is the density.

**MASS FLOW RATE**

The mass flow rate boundary condition sets the total mass flow through the boundary according to:

$$- \int_{\partial \Omega} d_{bc} \rho (u \cdot n) dS = m$$

where $d_{bc}$ (only present in the 2D Cartesian axis system) is the boundary thickness normal to the fluid-flow domain and $m$ is the total mass flow rate.

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary.
**STANDARD FLOW RATE**

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the boundary is set by the equation:

\[- \int_{\partial \Omega} \rho \mathbf{u} \cdot \mathbf{n} \, dS = Q_{sv}\]

where \(d_{bc}\) (only present in the 2D model Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, \(\rho_{st}\) is the standard density, and \(Q_{sv}\) is the standard flow rate. The standard density is defined by one of the following equations:

\[\rho_{st} = \frac{M_n}{V_n}\]

\[\rho_{st} = \frac{p_{st}M_n}{RT_{st}}\]

where \(M_n\) is the mean molar mass of the fluid, \(V_n\) is the standard molar volume, \(p_{st}\) is the standard pressure, \(R\) is the universal molar gas constant, and \(T_{st}\) is the standard temperature.

Equation 4-16 or Equation 4-17 is also enforced for compressible and incompressible flow, respectively, ensuring that the normal component of the viscous stress and the tangential component of the velocity are zero at the boundary.

---

**No Viscous Stress**

For this module, and in addition to the Pressure, No Viscous Stress Boundary Condition, the viscous stress condition sets the viscous stress to zero:

\[\left( \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) I \right) \mathbf{n} = 0\]

\[\left( \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right) \mathbf{n} = 0\]

using the compressible and the incompressible formulation, respectively.
The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

**Pressure, No Viscous Stress Boundary Condition**

The Pressure, No Viscous Stress boundary condition specifies vanishing viscous stress along with a Dirichlet condition on the pressure:

\[
\left( \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \mathbf{n} = 0, \quad p = p_0
\]

\[
\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} = 0, \quad p = p_0
\]

using the compressible and the incompressible formulation, respectively.

This boundary condition physically corresponds to flow entering from a large container. It is numerically stable and admits total control of the pressure level along the entire boundary; however, it can give artifacts on the boundary if the viscous stresses just downstream of the inlet are non-zero. In such situations there are two choices. Either move the boundary farther away to a location where the artifacts do not matter or use another stress type boundary condition present in the Boundary Stress feature.

While the Pressure, no viscous stress boundary condition is numerically more robust than the Normal stress condition (which also specifies the pressure), it is also theoretically over-constraining of the flow field (Ref. 4). This theoretical “flaw” is often ignored since it in most cases has no practical implication.

Inlet and Outlet for the node settings. Note that some modules have additional theory sections describing options available with that module.
Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude $f_0$, oriented in the negative normal direction:

\[
\left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -f_0\mathbf{n}
\]

\[
(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -f_0\mathbf{n}
\]

using the compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

\[
p = 2\mu \frac{\partial u_n}{\partial n} + f_0
\]

(4-17)

If $\partial u_n/\partial n$ is small, Equation 4-17 states that $p \approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure, No Viscous Stress condition (Ref. 4), but it is numerically less stable.

Pressure Boundary Condition

For single-phase flow, a mathematically correct natural boundary condition for outlets is

\[
(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n}
\]

(4-18)

This is a normal stress condition together with a no tangential stress condition. When $\mu > 0$ Equation 4-18 can be supplemented with a tangential velocity condition

\[
\mathbf{u} \cdot \mathbf{n} = 0
\]

(4-19)

If so, the no tangential stress condition is overridden. An issue with Equation 4-18 is that it does not strongly enforce outflow on the boundary. If the prescribed pressure is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier-Stokes equations as it is an issue for scalar transport equations solved along with Navier-Stokes equations. Hence, when applying the Pressure boundary condition at an outlet you can further constrain the outflow. With the Suppress backflow option
the normal stress is adjusted to keep

\[ \mathbf{u} \cdot \mathbf{n} \geq 0 \]  

**Equation 4-20** effectively means that the prescribed pressure is \( p_0 \) if \( \mathbf{u} \cdot \mathbf{n} \geq 0 \), but smaller at locations where \( \mathbf{u} \cdot \mathbf{n} < 0 \). This means that **Equation 4-20** does not completely prevent backflow, but the backflow is substantially reduced.

**Vacuum Pump Boundary Condition**

Vacuum pumps (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets/outlets nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a vacuum pump.

Also see **Vacuum Pump** for the node settings.

**Defining a Device at an Outlet**

In this case (see Figure 4-3), the device’s inlet is the interior face situated between the blue (cube) and green (circle) domains while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the **Pressure Boundary Condition** for outlets with the Suppress backflow option.
Here, $V_0$ is the flow rate across the boundary and $p_{\text{vacuum pump}}(V_0)$ is the static pressure function of flow rate for the vacuum pump. Equation 4-22 corresponds to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla \cdot \mathbf{u})$ vanishes.

In 2D the thickness in the third direction, $D_z$, is used to define the flow rate. Vacuum pumps are modeled as rectangles in this case.

\[
\mathbf{\hat{p}}_0 \leq p_{\text{vacuum pump}}(V_0)
\]

(4-22)

Figure 4-3: A vacuum pump at the outlet. The arrow represents the flow direction, the green circle represents the vacuum pump (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached vacuum pump.
Mass Sources for Fluid Flow

There are two types of mass sources in the Single-Phase Flow interface: point sources and line sources.

**POINT SOURCE**

A point source is theoretically formed by taking a mass injection/ejection, \( \dot{Q} \) (SI unit: \( \text{kg}/(\text{m}^3\cdot\text{s}) \)), in a small volume \( \delta V \) and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, \( \dot{q}_p \) (SI unit: \( \text{kg}/\text{s} \)), this can be expressed as

\[
\lim_{\delta V \to 0} \int \frac{\dot{Q}}{\delta V} = \dot{q}_p
\]

An alternatively way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

\[
\dot{q}_{p,\text{test}}(p)
\]

is added to a point in the geometry. As can be seen from Equation 4-23, \( \dot{Q} \) must tend to plus or minus infinity as \( \delta V \) tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that “point” refers to the physical representation of the source. A point source can therefore only be added to points in 3D models and to points on the symmetry axis in 2D axisymmetry models. Other geometrical points in 2D models represent physical lines.

The finite element representation of Equation 4-23 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point.
The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

**LINE SOURCE**

A line source can theoretically be formed by assuming a source of strength \( \dot{Q} \) (SI unit: \( \text{kg}/(\text{m}^3\cdot\text{s}) \)), located within a tube with cross-section area \( \delta S \) and then letting \( \delta S \) tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, \( \dot{q}_l \) (SI unit: \( \text{kg}/(\text{m}\cdot\text{s}) \)), this can be expressed as

\[
\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_l
\]

(4-24)

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects on the fluid resulting from the physical object volume are neglected.

The weak contribution

\[
\dot{q}_{l,\text{test}}(\rho)
\]

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry models. It can not, however, be added to geometrical lines in 2D since those represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

For feature node information, see Line Mass Source and Point Mass Source in the COMSOL Multiphysics Reference Manual.
Numerical Stability—Stabilization Techniques for Fluid Flow

The momentum equation (Equation 4-9 or Equation 4-11) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main fluid-flow features. To display this section, click the Show button ( ) and select Stabilization.

There are three types of stabilization methods available for Navier-Stokes—streamline diffusion, crosswind diffusion, and isotropic diffusion. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Batteries & Fuel Cells Module, these shared physics nodes are renamed as follows:

- The Line Mass Source node is available as two nodes, one for the fluid flow (Fluid Line Source) and one for the species (Species Line Source).
- The Point Mass Source node is available as two nodes, one for the fluid flow (Fluid Point Source) and one for the species (Species Point Source).

In the COMSOL Multiphysics Reference Manual:

- Numerical Stabilization
- Iterative

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 7) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 8). This is the
The time-scale tensor is the diagonal tensor presented in Ref. 9.

Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuska-Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier-Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

**Crosswind Diffusion**

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier-Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 8 with a shock capturing viscosity of the Hughes-Mallet type Ref. 7.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh.

Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

**Isotropic Diffusion**

Isotropic diffusion adds diffusion to the Navier-Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.
Solvers for Laminar Flow

The Navier-Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

**Nonlinear Solver**

The nonlinear solver depends if the model solves a stationary or a time-dependent problem.

**Stationary Solver**

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

**Time-Dependent Solver**

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also for the same reason, it suffices to update the Jacobian once per time-step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

---

Stationary Solver in the COMSOL Multiphysics Reference Manual
LINEAR SOLVER

The linearized Navier-Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure the equation system effectively shares many numerical properties with a saddle point system.

For small 2D models and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most non-singular systems and are very robust and also very fast for small models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and $N^2$ where $N$ is the number of degrees of freedom in the model. The default suggestion for large 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as $N$.

Geometric Multigrid (GMG) is used to accelerate GMRES. GMG needs smoothers but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. Pointwise smoothers, such as SOR, are not very efficient on anisotropic meshes.

The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher order elements, especially if Method in the SCGS settings is set to Mesh element lines. But there is no guarantee for this, so the default smoother for P2+P1 elements and P3+P2 elements is an SOR Line smoother. SOR Line handles mesh anisotropy, but does not formally address the saddle point character. It does however function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher order elements must either apply SCGS,
or use the Vanka smoother. The latter is the default suggestion for higher order elements, but it does not work optimally for anisotropic meshes.

In the *COMSOL Multiphysics Reference Manual*:
- Multigrid
- Direct
- Iterative
- SCGS
- SOR Line
- Vanka

**TIME-DEPENDENT SOLVER**

The default time-dependent solver for Navier-Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier-Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized-\(\alpha\) method instead. Generalized-\(\alpha\) is a solver which has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized-\(\alpha\) are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

**Pseudo Time Stepping for Laminar Flow Models**

A stationary formulation has per definition no time derivatives and Equation 4-11 reduces to:

\[
\rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-\rho \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}
\]  

(4-25)
Solving Equation 4-25 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative to Equation 4-25:

\[
\rho \left( \frac{\mathbf{u} - \text{nojac} \left( \mathbf{u} \right)}{\Delta t} \right) + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \left[ -\rho \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right] + \mathbf{F}
\]

where \( \Delta t \) is a pseudo time step. Since \( \mathbf{u} - \text{nojac} \left( \mathbf{u} \right) \) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size \( \Delta t \) of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step \( \Delta t \) can be chosen individually for each element based on the local CFL number:

\[
\Delta t = \text{CFL}_{\text{loc}} \frac{h}{|\mathbf{u}|}
\]

where \( h \) is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for \( \text{CFL}_{\text{loc}} \) is set to the built-in variable \( \text{CFLCMP} \). The automatic setting then suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases \( \text{CFL}_{\text{loc}} \) as the solution comes closer to convergence.

For details about the CFL regulator, see Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual.

The default manual expression is

\[
\text{CFL}_{\text{loc}} = \begin{cases} 
1.3 \min(niterCMP, 9) + 1, & \text{if } niterCMP > 20, \\
1.3 \min(niterCMP - 20, 9), & \text{if } niterCMP > 40, \\
0, & \text{otherwise}
\end{cases}
\]

(4-26)

The variable \( niterCMP \) is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. \( \text{CFL}_{\text{loc}} \) starts at 1.3 and increases by 30% each iteration until it reaches \( 1.3^9 \approx 10.6 \). It remains there until iteration number 20 at which it starts to
increase until it reaches approximately 106. A final increase after iteration number 40 then takes it to 1060. Equation 4-26 can for some advanced flows increase $CFL_{loc}$ too slowly or too quickly. $CFL_{loc}$ can then be tuned for the specific application.

**Discontinuous Galerkin Formulation**

Some boundary conditions are implemented using a discontinuous Galerkin formulation. These boundary conditions include:

- **Wall – Slip**
- **Periodic Flow Condition**
- **Flow Continuity**

The formulation used in the fluid-flow interfaces in COMSOL Multiphysics is the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 13.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter in COMSOL is implemented according to Ref. 14.

**Particle Tracing in Fluid Flow**

The Particle Tracing Module is available to assist with these types of modeling problems.

The model **Flow Past a Cylinder** (model library path `COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow`) demonstrates how to add and set up particle tracing in a plot group using the **Particle Tracing with Mass** node. It uses the predefined Khan-Richardson model for the drag force and neglects gravity and buoyancy forces.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and
then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton’s second law

$$m \frac{d^2 \mathbf{x}}{dt^2} = \mathbf{F}(t, \mathbf{x}, \frac{d\mathbf{x}}{dt})$$

where $\mathbf{x}$ is the position of the particle, $m$ the particle mass, and $\mathbf{F}$ is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expression have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 11). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$Re_p = \frac{|\mathbf{u} - \mathbf{u}_p|^2 r \rho}{\mu}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{u}_p$ the particle velocity, $r$ the particle radius, $\rho$ the fluid density, and $\mu$ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p|(|\mathbf{u} - \mathbf{u}_p|)(1.84 Re_p^{0.31} + 0.293 Re_p^{0.06})^{3.45}$$

References for the Single-Phase Flow, Laminar Flow Interfaces


The Boltzmann Equation, Two-Term Approximation Interface

This chapter describes the Boltzmann Equation, Two-Term Approximation interface, found under the Plasma branch when adding a physics interface.

In this chapter:

- The Boltzmann Equation, Two-Term Approximation Interface
- Theory for the Boltzmann Equation, Two-Term Approximation Interface
The Boltzmann Equation, Two-Term Approximation Interface

This interface is available for 1D models.

The Boltzmann Equation, Two-Term Approximation (be) interface ( ), found under the Plasma branch ( ) when adding a physics interface, studies the electron energy distribution function (EEDF) and calculates it from a set of collision cross sections for some mean discharge conditions. The interface is different because the geometry and mesh are fixed and automatically generated when the interface is added to a model. The $x$-axis represents an energy coordinate rather than physical space, enabling sets of collision cross sections to be loaded and the properties of the distribution function set. Additionally, electron source coefficients and transport properties can be computed. The Boltzmann Equation, Two-Term Approximation interface is intended as a preprocessing step before solving space-dependent models.

When this interface is added, these default nodes are also added to the Model Builder—Boltzmann Model and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click Boltzmann Equation, Two-Term Approximation to select physics from the context menu.

The Reduced Electric Fields study is available for this interface and described in the COMSOL Multiphysics Reference Manual.

**INTERFACE IDENTIFIER**

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

The default identifier (for the first interface in the model) is be.
**Domain Selection**

There is always only one domain for the interface. The position and length of the domain are automatically generated and rarely need to be changed.

**Cross Section Import**

Browse to a file containing a set of collision cross sections.

The file must follow the format documented in Importing Collision Cross-Section Data.

**Electron Energy Distribution Function**

Select an Electron energy distribution function—**Maxwellian** (the default), **Druyvesteyn**, **Generalized**, or **Boltzmann**.

- Select **Maxwellian** to assume a Maxwellian EEDF, which takes the form:

  \[
  f(\varepsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\varepsilon\beta_2/\varphi\right)
  \]

  where

  \[
  \beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{5/2}, \beta_2 = \Gamma(5/2)\Gamma(3/2)^{-1}
  \]

  and \(\varphi\) is the mean electron energy (eV), \(\varepsilon\) is the electron energy (eV) and \(\Gamma\) is the upper incomplete gamma function.

- Select **Druyvesteyn** to assume a Druyvesteyn EEDF, which takes the form:

  \[
  f(\varepsilon) = 2\varphi^{-3/2} \beta_1 \exp\left(-\varepsilon\beta_2/\varphi\right)^2
  \]

  where

  \[
  \beta_1 = \Gamma(5/4)^{3/2} \Gamma(3/4)^{5/2}, \beta_2 = \Gamma(5/4)\Gamma(3/4)^{-1}
  \]

- Select **Generalized** for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. If **Generalized** is selected, enter a value for the **Power law** \(g\) (dimensionless). The default is 1.5, and this number must be between 1 and 2. Mathematically, the EEDF takes the form:
where

\[ f(e) = g^{3/2} \beta_1 \exp\left(-e\beta_2/\varphi\right) \]

\[ \beta_1 = \Gamma(5/2g)^{-3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g)\Gamma(3/2g)^{-1}, 1 \leq g \leq 2 \]

So, when \( g = 1 \) the distribution function is Maxwellian and when \( g = 2 \) it is Druyvesteyn.

- Select Boltzmann to solve a two-term approximation to the Boltzmann equation. When selected, the EEDF is computed from a partial differential equation instead of by taking an assumed function. The two-term Boltzmann equation is a complicated, nonlocal integral equation.

**Boltzmann Properties**

This section is available when Boltzmann is selected as the Electron energy distribution function. These settings also enable available settings on the Boltzmann Model settings window.

- Select On or Off (the default) from the Electron-electron collisions list. If the ionization degree of the discharge is high then set this property to On.

Electron-electron collisions tend to make the distribution function more Maxwellian and they also increase the complexity of the problem.

- Select an option from the Secondary electron energy sharing list—Equal (the default) or Zero energy.

This describes how the energy is split between two electrons when an ionization collision occurs. If set to Equal, then both electrons take an equal energy after the collision. If the property is set to Zero energy then the secondary electron created in an ionization collision has zero energy and the ionizing electron carries all the excess energy.

- Select On or Off (the default) from the Oscillating field list. Only select On if the reduced angular frequency of the discharge is high, which is typically only true for microwave discharges. The reduced angular frequency is the ratio of the angular frequency and the neutral number density, \( \omega/N \).

**Dependent Variables**

The dependent variable (field variable) for the EEDF. The name can be changed but the names of fields and dependent variables must be unique within a model.
**Discretization**

To display this section, click the Show button ( ) and select Discretization. Select an EEDF—Linear, Quadratic (the default), Cubic, or Quartic. Specify the Value type when using splitting of complex variables—Real or Complex (the default).

- Show More Physics Options
- Domain, Boundary, and Pair Nodes for the Boltzmann Equation, Two-Term Approximation Interface
- Theory for the Boltzmann Equation, Two-Term Approximation Interface

### Domain, Boundary, and Pair Nodes for the Boltzmann Equation, Two-Term Approximation Interface

The Boltzmann Equation, Two-Term Approximation Interface has these domain, boundary, and pair nodes, listed in alphabetical order, 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).

- Argon Boltzmann Analysis: model library path Plasma_Module/Two-term_Boltzmann_Equation/boltzmann_argon
- Oxygen Boltzmann Analysis: model library path Plasma_Module/Two-term_Boltzmann_Equation/boltzmann_oxygen

In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. However, to add subnodes, right-click the parent node.

- Boltzmann Model
- Boundary Settings
- Collision
- Initial Values
• Zero Energy Flux
• Zero Probability

In the COMSOL Multiphysics Reference Manual:

- Continuity on Interior Boundaries
- Identity and Contact Pairs

Boltzmann Model

This node is available when Boltzmann is selected as the Electron Energy Distribution Function.

In the Boltzmann Model node, values for specific discharge parameters are set. The number of parameters needed depends on the property settings for the physics interface.

Domain Selection

There is always only one domain for the interface. The position and length of the domain are automatically generated and rarely needs to be changed.

Boltzmann Settings

• Enter a Gas temperature $T_g$ (SI unit: K). The default is 300 K. The gas temperature influences the amount of energy loss that an electron suffers during an elastic collision. The higher the gas temperature, the lower the energy loss for an electron during an elastic collision.

• If the Electron-electron collisions property is set to On in the Boltzmann Properties section, enter an estimate for the Electron density $n_e$ (SI unit: $1/m^3$).

There is a weak dependence on the electron density in Equation 5-1 which accounts for the screening of the Coulomb potential by space charge effects (Ref. 1).
• If the Electron-electron collisions property is set to On in the Boltzmann Properties section, enter an Ionization degree $\beta$ (dimensionless).

The ionization degree can have a significant effect on the shape of the electron energy distribution function. When the ionization degree is very low, the tail of the distribution function tends to decrease very rapidly. As the ionization degree increases, the distribution function tends to become more Maxwellian, resulting in a greater proportion of electrons with higher energies. This can have a profound effect on the rate coefficients for ionization and excitation collisions because of their high energy threshold.

• If the Oscillating field property is set to On in the Boltzmann Properties section, enter a Reduced angular frequency $\omega/N$ (SI unit: m$^3$/s). The default is $10^{-13}$ m$^3$/s.

If the reduced angular frequency is high, the proportion of electrons with high energies is substantially increased for the same mean electron energy. This is because in DC fields, collisional momentum transfer impedes electrons acquiring higher energies but high frequency fields have the opposite effect.

MOLE FRACTION SETTINGS

Specify the mole fraction of each of the target species in the set of collision cross sections.

Since the sum of all the mole fractions must be equal to one, select the Sum equals 1 check box to compute the mole fraction of the first species based on the mole fractions of all the other species. The Mole fraction of the first species cannot be edited when this option is selected.

Mole fraction. There are $N$ edit fields available for setting the mole fractions of each species, where $N$ is the total number of target species. Enter the Mole fraction expected to be observed in the discharge for each target species. The mole fraction of electronically excited species can have a strong effect on the shape of the electron energy distribution function.

Initial Values

The Initial Values node is only available if Boltzmann is selected as the Electron Energy Distribution Function. The Initial Values node allows you to set an initial guess for the mean electron energy, the Townsend reduced electric field, and the initial condition for a Lagrange multiplier.
**Domain Selection**

There is always only one domain for the interface. The position and length of the domain are automatically generated and should not be changed.

**Initial Values**

- Enter an **Initial mean electron energy** $e_0$ (SI unit: V). The default is 2 V. This should be equal to the mean electron energy of the first parameter in the parametric sweep. COMSOL Multiphysics constructs an initial guess at the EEDF by assuming a Maxwellian distribution function with the specified mean electron energy.

- Enter an **Initial Townsend reduced electric field** $T_d, 0$ (dimensionless). The default is 1 and this rarely needs to be changed. This is the initial reduced electric field used to compute the distribution function. In order to make the value intuitive to enter, the value is requested in units of Townsends.

- Enter an **Initial condition for lam** $\lambda_0$ (dimensionless). The default is $1 \times 10^{-27}$ and this rarely needs to be changed. This value is an initial guess for a Lagrange multiplier, which is used to force the mean electron energy to be equal to the specified mean electron energy.

**Collision**

Use the **Collision** node to add collisions to a model by entering a formula and some properties of the collision. The cross-section data can be entered manually or by loading it from a file.

Load in multiple cross sections from a file in the **Boltzmann Equation, Two-Term Approximation** settings. In this case, the collision features are automatically generated.
**DOMAIN SELECTION**

There is always only one domain for the interface. The position and length of the domain are automatically generated and should not be changed.

### COLLISION

Enter a **Formula** for the collision.

Select a **Collision type**— **Elastic** (the default), **Excitation**, **Attachment**, or **Ionization**.

- If **Elastic** is selected, enter a value for the **Electron mass ratio** \( m_r \) (dimensionless) (the ratio of the mass of the electron to the target species).
- Select **Excitation** for excitation reactions where the collision is inelastic. Enter the **Energy loss** \( \Delta \varepsilon \) (SI unit: V) for the reaction. This is also known as threshold energy for the reaction. Select this option for electronic excitation, vibrational and rotational excitation, and superelastic collisions. For superelastic collisions, the activation energy is negative.
- Select **Attachment** for collisions which result in the electron attaching to the target species, forming a negative ion. No user input is required.
- Select **Ionization** for electron impact reactions which result in secondary electrons being formed. Enter the **Energy loss** \( \Delta \varepsilon \) (SI unit: V) for the reaction. This is also known as threshold energy for the reaction.

### CROSS SECTION DATA

Enter the cross section data in two columns. Enter the **Electron energy** (SI unit: eV) and the **Collision cross section data** (SI unit: m\(^2\)). Also click the **Load from file** button ( ) to import data from a text file. The file must contain the two columns of data (**Electron energy** (SI unit: eV) in the first column and **Collision cross section data** (SI unit: m\(^2\)) in the second column).

**Boundary Settings**

The boundary conditions are always the same, **Zero energy flux** at \( \varepsilon = 0 \) and **Zero probability** as \( \varepsilon \to \infty \).
Zero Energy Flux

The Zero Energy Flux boundary condition should always be applied at $x = 0$. Physically the boundary condition specifies that no electrons can have energy less than zero electron volts.

**BOUNDARY SELECTION**
From the Selection list, choose the boundaries to define.

**PAIR SELECTION**
If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

Zero Probability

The Zero Probability boundary condition should always be applied at $\varepsilon = 100$. Physically the boundary condition states that there are no electrons with infinite energy. Instead of solving the problem in an infinite domain, the maximum value of $\varepsilon$ is chosen to be large enough so it does not affect the results. The default is $\varepsilon = 100$.

**BOUNDARY SELECTION**
From the Selection list, choose the boundaries to define.

**PAIR SELECTION**
If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.
Theory for the Boltzmann Equation, Two-Term Approximation Interface

The Boltzmann Equation, Two-Term Approximation Interface theory is described in this section:

- The Electron Energy Distribution Function
- Boltzmann Equation, Two-Term Approximation
- References for the Boltzmann Equation, Two-Term Approximation Interface

The Electron Energy Distribution Function

For computing the electron density and electron energy according to Equation 6-5 and Equation 6-6 transport properties and source coefficients are required. These coefficients can be calculated from collision cross-section data and the (unknown) electron energy distribution function (EEDF). The equation formulation used in the interface depends on whether the EEDF is an assumed function (Maxwellian, Druyvesteyn or Generalized) or is to be explicitly computed by the Boltzmann equation, using the two-term approximation.

Obtaining a physical solution for a fluid model of a plasma largely depends on how self-consistently the transport properties and source coefficients are calculated. By solving the two-term Boltzmann equation, maximum consistency is obtained between the kinetic and fluid description of the electron dynamics.

Solving the Boltzmann equation also makes it possible to calculate the drift velocity. The drift velocity is an important quantity because it depends on all the collisions which make up the plasma chemistry. The drift velocity is easy to measure, and comparing the experimental and simulated drift velocity is therefore straightforward. Indeed, collision cross sections are often inferred from drift velocity data.

Verifying that the experimental drift velocity agrees with the computed drift velocity is a good indicator that a given set of cross sections are correct. This interface makes it easy to compare the computed drift velocity to experimental data. A treatise on experimental measurements of the drift velocity is available in Ref. 2.

Consider the following expression
where the following definitions apply

\[
\beta_1 = \Gamma(5/2g)^{3/2}\Gamma(3/2g)^{-5/2}, \quad \beta_2 = \Gamma(5/2g)\Gamma(3/2g)^{-1}, \quad 1 \leq g \leq 2
\]

and \( \varphi \) is the mean electron energy. Depending on the value of the variable, \( g \), the distribution function is either Maxwellian (\( g = 1 \)), Druyvesteyn (\( g = 2 \)), or Generalized (\( 1 < g < 2 \)). Mathematically, the distribution functions are defined as:

**MAXWELLIAN EEDF**

\[
f(\varepsilon) = \varphi^{-3/2}\beta_1 \exp\left(-\left(\varepsilon\beta_2/\varphi\right)^2\right)
\]

**DRUYVESTEYN EEDF**

\[
f(\varepsilon) = 2\varphi^{-3/2}\beta_1 \exp\left(-\left(\varepsilon\beta_2/\varphi\right)^2\right)
\]

**GENERALIZED EEDF**

\[
f(\varepsilon) = g\varphi^{-3/2}\beta_1 \exp\left(-\left(\varepsilon\beta_2/\varphi\right)^2\right)
\]

The Boltzmann equation describes the evolution of a distribution function, \( f \), in six-dimensional phase space:

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{e}{m} (\mathbf{E} \cdot \nabla \mathbf{v}) f = C[f].
\]

To be able to solve the Boltzmann equation and thus compute the EEDF, drastic simplifications are necessary. A common approach is to expand the distribution function in spherical harmonics. For high precision six or more terms might be needed. If the EEDF can be assumed almost spherically symmetric, the series can be truncated.
after the second term. The EEDF becomes symmetric because in elastic collisions with neutral atoms the direction of motion of the electrons is changed and their loss of energy is small due to large mass difference. The two-term approximation is valid for all values of reduced electric field (the ratio of the electric field to the number density of the background gas) if inelastic scattering can be neglected, there is no minimum in the cross section and the cross section for momentum transfer is related to the electron energy by a power-law dependence, Ref. 3.

When the Boltzmann equation option is selected, it becomes necessary to solve a 1D reaction/convection/diffusion equation to compute the EEDF. The equation is somewhat special because the source term is nonlocal and the convection and diffusion coefficients depend on the integral of the solution. The stationary two-term Boltzmann equation, including the effects of electron-electron collisions is:

\[
\frac{\partial}{\partial t} (W f - D \frac{\partial f}{\partial W}) = S
\]

where

\[
W = -\gamma \varepsilon^2 \sigma_e - 3a \left( \frac{n_e}{N_n} \right) A_1
\]

\[
D = \frac{\gamma (E \beta N_n)^2}{\beta} \left( \frac{\varepsilon}{\sigma_m} \right) + \frac{y_k T}{q} \varepsilon^2 \sigma_e + 2a \left( \frac{n_e}{N_n} \right) (A_2 + \varepsilon^{3/2} A_3)
\]

The following definitions apply

\[
a = \frac{q^2 \gamma E}{24 \pi \varepsilon_0} \ln \Lambda
\]

\[
\Lambda = \frac{12 \pi (2 \varepsilon_0 q E / 3)^{3/2}}{q^3 n_e^{1/2}}
\]

(5-1)

\[
\sigma_m = \sum_{k = all} x_k \sigma_k
\]

\[
\sigma_c = \sum_{k = elastic} 2 \left( \frac{m_e}{M} \right) x_k \sigma_k
\]
\[ \sigma_m = \sigma_m + \frac{\lambda}{\epsilon^{1/2}} \]

\[ A_1 = \int_0^\epsilon u^{1/2} f(u) du \]

\[ A_2 = \int_0^\epsilon u^{3/2} f(u) du \]

\[ A_3 = \int_\epsilon^\infty f(u) du \]

Here:
- \( \gamma = (2q/m_e)^{1/2} \) (SI unit: \( C^{1/2}/kg^{1/2} \))
- \( m_e \) is the electron mass (SI unit: kg)
- \( \epsilon \) is energy (SI unit: V)
- \( \sigma_\epsilon \) is the total elastic collision cross section (SI unit: m\(^2\))
- \( \sigma_m \) is the total collision cross section (SI unit: m\(^2\))
- \( q \) is the electron charge (SI unit: C)
- \( \varepsilon_0 \) is the permittivity of free space (SI unit: F/m)
- \( T \) is the temperature of the background gas (SI unit: K)
- \( k_b \) is the Boltzmann constant (SI unit: J/K)
- \( n_e \) is the electron density (SI unit: 1/m\(^3\))
- \( N_n \) is the background gas density (SI unit: 1/m\(^3\))
- \( \Lambda \) is the Coulomb logarithm, and
- \( M \) is the mass of the target species (SI unit: kg).

The source term, \( S \) represents energy loss due to inelastic collisions. Because the energy loss due to an inelastic collision is quantized, the source term is nonlocal in energy space. The source term can be decomposed into four parts where the following definitions apply:

\[ S = \sum_{k = \text{inelastic}} C_k - \gamma k \epsilon^{1/2} f \]

\[ C_k = \text{excitation} = -\gamma k \left[ \varepsilon \sigma_k (\epsilon) f(\epsilon) - (\epsilon + \Delta\epsilon_k) \sigma_k (\epsilon + \Delta\epsilon_k) f(\epsilon + \Delta\epsilon_k) \right] \]
where \( x_k \) is the mole fraction of the target species for reaction \( k \), \( \sigma_k \) is the collision cross section for reaction \( k \), \( \Delta \varepsilon_k \) is the energy loss from collision \( k \), and \( \delta \) is the delta function at \( \varepsilon = 0 \). The term, \( \lambda \), is a scalar valued renormalization factor which ensures that the EEDF has the following property:

\[
\int_0^\infty f_\varepsilon^{1/2} d\varepsilon = 1
\]

(5-2)

An ODE is implemented to solve for the value of \( \lambda \) such that Equation 5-2 is satisfied. The rate coefficients are computed from the EEDF by way of the following integral:

\[
k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon)f(\varepsilon)d\varepsilon
\]

The mean electron energy is defined by the integral:

\[
\bar{\varepsilon} = \int_0^\infty f_\varepsilon^{3/2} d\varepsilon
\]

(5-3)

In order to set the mean electron energy to a specific setpoint, a second Lagrange multiplier is introduced to solve for the reduced electric field, such that Equation 5-3 is satisfied. The weak form of the constraint is:

\[
\left( \int_0^\infty f_\varepsilon^{3/2} d\varepsilon - v_{sp} \right) \left( \frac{E}{N_n} \right) = 0
\]

where tilde denotes test function. The drift velocity is computed from the following integral:

\[
w = \left( \frac{1}{3} \right) \left( \frac{E}{N_n} \right) \int_0^\infty \varepsilon \frac{\sigma_m(\varepsilon)}{\varepsilon} d\varepsilon
\]

The drift velocity is an important quantity for two reasons. Firstly, it provides a convenient way of comparing the results of the Boltzmann equation to experimental
data. The second reason is that it allows the Townsend coefficients to be computed using:

$$\alpha_k = \frac{r_k}{w}$$

When the distribution function is assumed, the reduced electric field must be computed in a completely different manner. The reduced electric field is not required to compute the rate coefficients or transport properties. It only needs to be calculated so that the Townsend coefficients and the drift velocity can be computed. The following expression is defined:

$$\left(\frac{E}{N_n}\right) = \frac{Y}{\mu_e N_n}$$

where

$$Y = \sum_k x_k k \Delta e_k$$

and $\Delta e_k$ is the energy loss for collision $k$. If the collision is elastic, the energy loss is defined as:

$$\Delta e_k = 2e\left(\frac{m_e}{M}\right)$$

A plot of the drift velocity for different distribution functions versus the reduced electric field for oxygen is shown in Figure 5-1. Experimental data is also included in the plot.

The reduced transport properties are computed using the following integrals:

$$\mu_e N_n = -\frac{\gamma}{3} \int_0^\infty \frac{e}{\sigma_m} \frac{\partial f}{\partial e} de$$

$$D_e N_n = \left(\frac{\gamma}{3}\right) \int_0^\infty \frac{e}{\sigma_m} \frac{\partial f}{\partial e} de$$

$$\mu_e N_n = -\frac{\gamma}{3\sigma} \int_0^\infty \frac{e^2}{\sigma_m} \frac{\partial f}{\partial e} de$$
Figure 5-1: Plot of experimental and computed drift velocity for different distribution functions.

The computed transport coefficients have little dependence on the type of EEDF. However, the rate coefficients for excitation and ionization processes are highly dependent on the shape of the EEDF, due to the exponential drop off in the population of electrons at energies exceeding the activation threshold. Figure 5-2 plots the ionization rate coefficient for oxygen for the types of distribution function.
Figure 5-2: Plot of ionization coefficient vs. mean electron energy for different distribution functions.

References for the Boltzmann Equation, Two-Term Approximation Interface


This chapter describes the underlying electron transport theory for the Drift Diffusion interface, found under the Plasma branch when adding a physics interface.

In this chapter:

- The Drift Diffusion Interface
- Theory for the Drift Diffusion Interface
The Drift Diffusion Interface

The Drift Diffusion (dd) interface ( ), found under the Plasma branch ( ) when adding a physics interface, solves for the electron density and mean electron energy for any type of plasma. A wide range of boundary conditions are available to handle secondary emission, thermionic emission, and wall losses.

When this interface is added, these default nodes are also added to the Model Builder—Drift Diffusion Model, Insulation (the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Drift Diffusion to select physics from the context menu.

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

The default identifier (for the first interface in the model) is dd.

DOMAIN SELECTION
The default setting is to include All domains in the model to define the dependent variables and the equations. To choose specific domains, select Manual from the Selection list.

ELECTRON PROPERTIES
The following check boxes are available—Use reduced electron transport properties, Compute tensor electron transport properties, Include thermal diffusion, or Fix mean electron energy.

Use Reduced Electron Transport Properties
Select the Use reduced electron transport properties check box to specify the electron mobility, diffusivity, energy mobility and energy diffusivity in reduced form. The neutral number density is then specified in the Drift Diffusion Model node. The electron transport properties are computed from the reduced transport properties using:
where $N_n$ is the user-defined neutral number density.

It is sometimes more convenient to use reduced transport properties, since they can be output from The Boltzmann Equation, Two-Term Approximation Interface.

*Compute Tensor Electron Transport Properties*
Select the *Compute tensor electron transport properties* check box to automatically compute the tensor form of the electron mobility, diffusivity, energy mobility and energy diffusivity when a static magnetic field is present. In this case the magnetic flux density is specified in the Drift Diffusion Model feature.

*Include Thermal Diffusion*
Select the *Include thermal diffusion* check box to add an additional term to the definition of the electron current due to gradients in the electron diffusivity. If the diffusivity is a constant then including this does not effect the solution. It is only necessary to include this term if the electron diffusivity is a function of the electron temperature, and there are significant gradients in the electron temperature.

*Fix Mean Electron Energy*
Select the *Fix mean electron energy* check box to fix the mean electron energy to its initial value. This can be useful in some situations because the strong coupling between the mean electron energy and the electromagnetic fields is removed. This allows for non-self-consistent models to be created quickly, since problems where the mean electron energy is fixed are easier to solve numerically.

**STABILIZATION**
If the *Equation formulation* is set to Log then the solver can run into difficulties as the electron density or electron energy density approach zero. The *Source stabilization* check box (selected by default) adds an additional source term to the equation for the electron density and electron energy density. In the $\zeta$ field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25-0.5. For information on stabilization see Stabilization.
ADVANCED SETTINGS

Use the Equation formulation to choose whether to solve the drift-diffusion equations in log or linear form. The default is set to log which means that COMSOL Multiphysics solves for the log of the electron density and electron energy density. This is generally more numerically stable than the linear form of the equations.

DEPENDENT VARIABLES

The dependent variables (field variables) for the Electron density and Electron energy density. The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

To display this section, click the Show button ( ) and select Discretization. Select a Log of electron density—Linear (the default), Quadratic, Cubic, or Quartic. Select a Log of electron energy density—Linear (the default), Quadratic, Cubic, or Quartic. Specify the Value type when using splitting of complex variables—Real or Complex (the default).

Drift Diffusion Tutorial: model library path
Plasma_Module/Direct_Current_Discharges/drift_diffusion_tutorial

Domain, Boundary, and Pair Nodes for the Drift Diffusion Interface

The Drift Diffusion Interface has these domain, boundary, and pair nodes, listed in alphabetical order, 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. However, to add subnodes, right-click the parent node.
Drift Diffusion Model

The Drift Diffusion Model adds the equations for electron transport in a plasma. Specify expressions for the electron diffusivity, mobility, electron energy diffusivity and electron energy mobility. There are also model inputs for the electric potential and collisional power loss.

**DOMAIN SELECTION**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

The boundary conditions are used for the electron density and mean electron energy, which make it easy to specify how the electrons interact with the wall. Secondary emission, thermionic emission and reflection can all be specified.

It is also possible to impose the specific value of the electron density or mean electron energy on a boundary. This, however, is not recommended as imposing such a value on a solid surface tends not to fit the physics of the interaction between a solid surface and electrons.

In the COMSOL Multiphysics Reference Manual:

- Continuity on Interior Boundaries
- Identity and Contact Pairs

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<table>
<thead>
<tr>
<th>Drift Diffusion Model</th>
<th>General Power Deposition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Values</td>
<td>Inductive Power Deposition</td>
</tr>
<tr>
<td>Electron Density and Energy</td>
<td>Insulation</td>
</tr>
<tr>
<td>Electron Outlet</td>
<td>Microwave Power Deposition</td>
</tr>
<tr>
<td>Electron Production Rate</td>
<td>Velocity</td>
</tr>
<tr>
<td>Flux</td>
<td>Wall</td>
</tr>
</tbody>
</table>
MODEL INPUTS
This section contains fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs are listed here.

- **Electric potential** V (SI unit: V). Used to compute the electric field which results in migration of the electrons.
- **Collisional power loss** $S_{en}$ (SI unit: W/m³). Represents the energy loss due to elastic and inelastic collisions.
- When the Use Reduced Electron Transport Properties check box is selected, chose **Neutral number density** $N_n$ (SI unit: 1/m³) to compute the electron transport.
- When the Compute Tensor Electron Transport Properties check box is selected, chose **Magnetic flux density** $B$ (SI unit: T) to compute the tensor form of the electron transport properties when a static magnetic field is present.

The electric potential typically comes from an Electrostatics interface and the collisional power loss is typically defined by The Heavy Species Transport Interface.

ELECTRON DENSITY AND ENERGY
This section is not available if the Compute Tensor Electron Transport Properties check box is selected.

For all other choices, select an option from the Electron transport properties list— Specify Mobility Only (the default), Specify All, or Use Lookup Tables.

The other transport properties are computed using Einstein’s relation, see Tensor Transport Properties for more details.

Specify Mobility Only
When no check boxes, or the Include Thermal Diffusion or Fix Mean Electron Energy check boxes are selected, and if Specify mobility only is selected, enter a value or expression for the **Electron mobility** $\mu_e$ (SI unit: m²/(V·s)). Select Isotropic, Diagonal, Symmetric or Anisotropic based on the model. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

$$D_e = \mu_e T_e, \quad \mu_e = \left(\frac{5}{3}\right) \frac{\delta}{2} \mu_e, \quad D_e = \mu_e T_e$$  \hspace{1cm} (6-1)
If the Use Reduced Electron Transport Properties check box is selected, enter the 
**Reduced electron mobility** $\mu_e N_n$ (SI unit: sA/(m$^3$kg)). The actual electron mobility 
is then computed by dividing the reduced electron mobility by the neutral number 
density. The electron diffusivity, energy mobility and energy diffusivity are then 
computed as in Equation 6-1.

**Specify All**

If Specify all is selected, enter values or expressions for all of the properties, which can 
be either scalars or tensors. The appropriate values for the transport properties can be 
computed with The Boltzmann Equation, Two-Term Approximation Interface. For all 
of the properties, select Isotropic, Diagonal, Symmetric or Anisotropic from the list based 
on the model, then enter values or expressions for all of these properties:

- **Electron mobility** $\mu_e$ (SI unit: m$^2$/(V·s))
- **Electron diffusivity** $D_e$ (SI unit: m$^2$/s)
- **Electron energy diffusivity** $D_{en}$ (SI unit: m$^2$/s)
- **Electron energy mobility** $\mu_{en}$ (SI unit: m$^2$/(V·s))

If the Use Reduced Electron Transport Properties check box is selected, then enter:

- **Reduced electron mobility** $\mu_e N_n$ (SI unit: s·A/(m$^3$kg))
- **Reduced electron diffusivity** $D_e N_n$ (SI unit: 1/(m·s))
- **Reduced electron energy diffusivity** $D_{en} N_n$ (SI unit: 1/(m·s))
- **Reduced electron energy mobility** $\mu_{en} N_n$ (SI unit: s·A/(m$^3$kg))

**Use Lookup Tables**

If Use lookup tables is selected, enter or load a lookup table with the transport 
properties as listed above versus mean electron energy (eV).

---

If the Use Reduced Electron Transport Properties check box is selected, the 
appropriate values for the transport properties can be computed with 
The Boltzmann Equation, Two-Term Approximation Interface and 
written out to a text file. The text file can then be loaded in for each 
electron transport property.

**DC ELECTRON MOBILITY**

This section is available if the Compute Tensor Electron Transport Properties check 
box is selected. Enter a value for the **DC electron mobility** $\mu_{dc}$ (SI unit: m$^2$/(V·s)).
The section is also available when both the Compute Tensor Electron Transport Properties and the Use Reduced Electron Transport Properties check boxes are chosen. Then enter a value or expression for the Reduced DC electron mobility, \( \mu_{dc} \) (SI unit: \( \text{m}^2/(\text{V} \cdot \text{s}) \)).

**Initial Values**

The Initial Values node adds initial values for the electron density and mean electron energy.

**Domain Selection**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

**Initial Values**

Enter values or expressions for the initial value of the Initial electron density \( n_{e,0} \) (SI unit: \( \text{1/m}^3 \)) and Initial mean electron energy \( e_0 \) (SI unit: \( \text{V} \)). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess can be set to the expected value the easier it is to find a solution.

**Electron Production Rate**

Use the Electron Production Rate node to add sources and sinks to the number density of electrons. Ionization processes lead to an increase in the number density of electrons. Similarly, attachment leads to a decrease in the number density of electrons. A production rate for new electrons can be specified with this feature.

**Domain Selection**

From the Selection list, choose the domains to define.

**Electron Production Rate**

Select or enter a value for a Production rate \( R_e \) (SI unit: \( \text{1/m}^3 \cdot \text{s} \)) of new electrons. The value typically comes from The Heavy Species Transport Interface.
General Power Deposition

Use the General Power Deposition to add an arbitrary heat source to the electrons.

Domain Selection

From the Selection list, choose the domains to define any heat sources due to induction currents.

General Power Deposition

Enter a value or expression for the General heat source $Q$ (SI unit: W/m$^3$). This could be a constant number or come from another physics interface.

Velocity

Use the Velocity node to include the effect of convection due to a moving gas. In nearly all practical situations, convection of electrons due to gas movement is negligible.

Domain Selection

From the Selection list, choose the domains to define convection due to a computed gas velocity.

Velocity

The Velocity field $\mu$ (SI unit: m/s) value or expression can be user-defined or come from another physics interface, typically Laminar Flow.

Inductive Power Deposition

The Inductive Power Deposition node requires a license for the AC/DC Module. Use it to add a heat source to the electrons from induction currents. This is typically used in inductively coupled plasmas.

Domain Selection

From the Selection list, choose the domains to define any heat sources due to induction currents.

Inductive Power Deposition

Enter a Heat source $Q$ (SI unit: W/m$^3$) for the electrons due to induction currents. Typically this comes from a Magnetic Fields interface.
Microwave Power Deposition

The Microwave Power Deposition node requires a license for the RF Module. Use it to add microwave heating to the electrons. This is typically used in wave heated discharges.

**DOMAIN SELECTION**

From the Selection list, choose the domains to define any heat sources due to electromagnetic waves.

**MICROWAVE POWER DEPOSITION**

Enter a Heat source \( Q \) (SI unit: \( \text{W/m}^3 \)) for the electrons due to electromagnetic waves. This typically comes from an Electromagnetic Waves interface.

**Insulation**

Use the Insulation boundary condition for boundaries which correspond to inlets or outlets for the background gas and it is the default boundary condition for the Drift Diffusion interface. It is also available on the Pairs menu. This boundary condition requires no user input. The boundary condition sets the normal component of the electron and electron energy flux to zero:

\[
-n \cdot \Gamma_e = 0 \quad \text{and} \quad -n \cdot \Gamma \epsilon = 0
\]

**BOUNDARY SELECTION**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific boundaries or select All boundaries as required.

**PAIR SELECTION**

If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**Electron Density and Energy**

The Electron Density and Energy boundary condition fixes the electron density to a specific number density or the mean electron energy to a specific energy. It is also
available on the **Pairs** menu. This boundary condition should, in general, be avoided in favor of the **Wall** boundary condition.

\[ n_e = n_{ew} \quad \text{and} \quad \bar{\varepsilon} = \bar{\varepsilon}_0 \]

Due to the fact that the log of the electron density is solved for, specifying an electron density of zero is not allowed.

---

**BOUNDARY SELECTION**

From the **Selection** list, choose the boundaries to define.

**PAIR SELECTION**

If this node is selected from the **Pairs** menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**ELECTRON DENSITY AND ENERGY**

Select the **Fix electron density** check box to enter a value for the **Electron density at the wall** \( n_{ew} \) (SI unit: \( 1/m^3 \)).

Select the **Fix mean electron energy** check box to enter a value for the **Mean electron energy at the wall** \( e \) (SI unit: \( V \)).

**Wall**

Use the **Wall** boundary condition when the plasma is in contact with a solid surface. This also allows for secondary and thermionic emission effects from the solid surfaces.

Use the **Wall** boundary condition to describe how the electrons interact with the wall.

---

**DOMAIN SELECTION**

From the **Selection** list, choose the domains to define.
GENERAL WALL SETTINGS
Enter a value for the Reflection coefficient \( r_e \) (dimensionless) on the selected boundaries. This must be a number between 0 and 1.

The Include migration effects check box should be checked if the electron flux to the wall is due to the electric field. This is usually not the case since the plasma potential is positive with respect to the walls so the electron flux to the wall due to the electric field is zero. In models where the electrostatic field changes very rapidly (like with dielectric barrier discharges for example) the electron flux to the wall can be due to the electric in which case this option should be activated.

ELECTRON DENSITY WALL SETTINGS
The Use wall for electron density check box is selected by default and deactivates the wall boundary condition for the electron density.

Select or enter a value for the Secondary emission flux (SI unit: \( 1/\text{m}^2\text{-s} \)). The secondary emission flux can either be a user-defined expression or come from another physics interface, typically The Heavy Species Transport Interface.

Select or enter a value for the Thermal emission flux (SI unit: \( 1/\text{m}^2\text{-s} \)). If electrons are being emitted from the wall due to thermal emission then enter an expression for the thermionic flux. Typically this only occurs when the wall is at a very high temperature.

ELECTRON ENERGY WALL SETTINGS
The Use wall for electron energy check box is selected by default and deactivates the wall boundary condition for the electron energy. This is useful in order to use the wall condition for the electron density but impose the value of the mean electron energy on the same boundaries.

Select or enter a value for the Secondary emission energy flux, which can either be a user-defined expression or come from another interface, typically The Heavy Species Transport Interface.

Select or enter a value for the Mean thermionic energy. If electrons are being emitted from the wall due to thermionic emission then enter an expression for the mean energy of the emitted electrons. The mean electron energy of the emitted electrons is usually a function of the work function of the surface.
**Flux**

Use the Flux node to select whether the boundary condition is imposed for electron density or electron energy or both. The wall boundary condition should be used in preference to the flux boundary conditions for walls. A user-defined electron Flux can be specified by the following:

\[ -\mathbf{n} \cdot \Gamma_e = \Gamma_{e,\text{in}} \quad \text{and} \quad -\mathbf{n} \cdot \Gamma_{e\text{,en}} = \Gamma_{e,\text{en}} \]

**Boundary Selection**
From the Selection list, choose the boundaries to define.

**Pair Selection**
If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

**Flux**
Select the Use flux for electron density check box to activate the boundary condition for electron density. Then enter a value for the Electron density influx \( r_e \) (SI unit: \(1/(m^2 \cdot s))\).

Select the Use flux for electron energy density to activate the boundary condition for electron energy. Then enter a value for the Electron energy density influx \( r_{e\text{en}} \) (dimensionless).

**Electron Outlet**
Use the Electron Outlet boundary condition for boundaries which correspond to outlets for the background gas. This boundary condition requires no user input. The boundary condition sets the normal component of the electron and electron energy flux to zero:

\[ -\mathbf{n} \cdot \Gamma_e = 0 \quad \text{and} \quad -\mathbf{n} \cdot \Gamma_{e\text{,en}} = 0 \]

**Boundary Selection**
From the Selection list, choose the boundaries to define.
Theory for the Drift Diffusion Interface

The Drift Diffusion Interface theory is described in this section:

- Introduction to Drift Diffusion Theory
- Electron Transport Theory
- Source Coefficients
- Stabilization
- Tensor Transport Properties
- The Wall Boundary Condition
- The Insulation Boundary Condition
- The Electron Density and Energy Boundary Condition
- Reference for the Drift Diffusion Interface

Introduction to Drift Diffusion Theory

In general, electron transport is described by the Boltzmann equation, which is a non-local continuity equation in phase space \((\mathbf{r}, \mathbf{u})\). The Boltzmann equation is an extremely complicated integrodifferential equation and solving it in an efficient manner is not currently possible. The Boltzmann equation can be approximated by fluid equations by multiplying by a weighting function and then integrating over velocity space. This reduces the governing equations to a three-dimensional, time-dependent problem. The fluid equations describe the electron number density, the mean electron momentum and the mean electron energy as a function of configuration space and time. The rate of change of the electron density is described by:

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot \mathbf{\Gamma}_e = R_e
\]

(6-2)

where \(n_e\) is the electron density, \(\mathbf{\Gamma}_e\) is the electron flux vector and \(R_e\) is either a source or a sink of electrons. The rate of change of the electron momentum is described by:

\[
\frac{\partial}{\partial t}(n_e m_e \mathbf{u}_e) + \nabla \cdot n_e m_e \mathbf{u}_e \mathbf{u}_e^T = - (\nabla \cdot \mathbf{p}_e) + q n_e \mathbf{E} - n_e m_e \mathbf{u}_e \mathbf{v}_m
\]

(6-3)
where $m_e$ is the electron mass (SI unit: kg), $u_e$ is the drift velocity of the electrons (SI unit: m/s), $p_e$ is the electron pressure tensor (SI unit: Pa), $q$ is the electron charge (SI unit: C), $E$ is the electric field (SI unit: V/m) and $v_m$ is the momentum transfer frequency (SI unit: 1/s). The rate of change of the electron energy density is described by:

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e + E \cdot \Gamma_e = R_e
\]  

(6-4)

where $n_e$ is the electron energy density (V/m$^3$) and $R_e$ is the energy loss or gain due to inelastic collisions (V/m$^3$ s). The expression for the flux, $\Gamma_e$ in Equation 6-2 is derived from the momentum conservation, Equation 6-3. Under the assumptions that the ionization and attachment frequencies and also the angular frequency are much less than the momentum transfer frequency, the first term on the left hand side of Equation 6-3 can be neglected. Under the assumption that the electron drift velocity is smaller than the thermal velocity, the second term on the left hand side of Equation 6-3 can also be neglected. For a Maxwellian distribution the pressure term, $p_e$ can be replaced using the equation of state:

\[ p_e = n_e k_B T_e \]

where $I$ is the identity matrix and $T_e$ is the electron temperature. With these assumptions an expression for the electron drift velocity can be derived:

\[ u_e = -\frac{k_B}{m_e v_m} \nabla T_e - \frac{k_B T_e}{n_e m_e v_m} \nabla n_e - \frac{q}{m_e v_m} E. \]

Defining the electron flux as:

\[ \Gamma_e = n_e u_e = - (\mu_e \cdot E) n_e - \nabla (D_e n_e) \]

where the electron mobility, $\mu_e$ (SI unit: m$^2$/(V s)) is defined as:

\[ \mu_e = \frac{q}{m_e v_m} \]

and the electron diffusivity, $D_e$ (SI unit: m$^2$/s) is defined as:

\[ D_e = \frac{k_B T_e}{m_e v_m} \]
The drift-diffusion approximation is suitable when the gas pressure is above about 1 mtorr (0.133 Pa) and the reduced electric field is not too high (typically less than 500 Townsends). Furthermore, the number density of charged species should be much less than the number density of the background gas. In other words, the discharge must be *weakly ionized*. The plasma must also be *collisional* which means that the mean free path between electrons and the background gas must be much less than the characteristic dimension of the system. This means the drift diffusion approximation is not suitable for modeling fusion plasmas.

The Drift Diffusion interface solves one equation for the electron density and one for the electron energy density.

### Electron Transport Theory

The equation for the electron density is given by

\[
\frac{\partial}{\partial t} n_e + \nabla \cdot \Gamma_e = R_e - (\mathbf{u} \cdot \nabla) n_e
\tag{6-5}
\]

\[
\Gamma_e = - (\mathbf{\mu}_e \cdot \mathbf{E}) n_e - \nabla (\mathbf{D}_e n_e)
\]

Here (the subscript \(e\) refers to an electron):

- \(n_e\) denotes the electron density (SI unit: \(1/m^3\))
- \(R_e\) is the electron rate expression (SI unit: \(1/(m^3\cdot s)\))
- \(\mathbf{\mu}_e\) is the electron mobility which is either a scalar or tensor (SI unit: \(m^2/(V\cdot s)\))
- \(\mathbf{E}\) is the electric field (SI unit: \(V/m\))
- \(\mathbf{D}_e\) is the electron diffusivity which is either a scalar or a tensor (SI unit: \(m^2/s\)), and
- \(\mathbf{u}\) is the neutral fluid velocity vector (SI unit: \(m/s\)). This usually comes from a Navier-Stokes interface and in the case of electrons is almost always negligible.

The *electron energy density* is given by the following equation

\[
\frac{\partial}{\partial t} \varepsilon_e + \nabla \cdot \Gamma_e + \mathbf{E} \cdot \Gamma_e = R_e - (\mathbf{u} \cdot \nabla) \varepsilon_e
\tag{6-6}
\]
\[ \Gamma_e = -(\mu_e \cdot \mathbf{E})n_e - \nabla(D_e n_e) \]

where (the subscript \( \varepsilon \) refers to electron energy):

- \( n_e \) is the electron energy density (SI unit: \( \text{V/m}^3 \))
- \( R_e \) is the energy loss/gain due to inelastic collisions (SI unit: \( \text{V/(m}^3\cdot\text{s}) \))
- \( \mu_e \) is the electron energy mobility which is either a scalar or a tensor (SI unit: \( \text{m}^2/(\text{V} \cdot \text{s}) \))
- \( \mathbf{E} \) is the electric field (SI unit: \( \text{V/m} \)), and
- \( D_e \) is the electron energy diffusivity (SI unit: \( \text{m}^2/\text{s} \)).

The mean electron energy, \( \bar{\varepsilon} \) (SI unit: \( \text{V} \)) is computed through the expression

\[ \bar{\varepsilon} = \frac{\varepsilon}{n_e} \]  \hspace{1cm} (6-7)

Because of the high degree of nonlinearity inherent in the drift diffusion equation, the electron number density can span 10 orders of magnitude over a very small distance. In this region (the plasma sheath), the difference in the mobility and diffusivity between the ions and electrons creates a separation of space charge. This in turn produces a large electric field which can lead to a substantial increase in the mean electron energy. The best way of handling with this from a numerical point of view is to solve for the log of the electron number and energy density. This also prevents a divide by zero from occurring when equation Equation 6-7 is evaluated. So, letting \( N_e = \ln n_e \), equation Equation 6-5 becomes

\[ e^N \frac{\partial}{\partial t}(N_e) + \nabla \cdot \left[ -e^N(\mu_e \cdot \mathbf{E}) - e^N(\nabla(D_e N_e)) \right] = R_e - (\mathbf{u} \cdot \nabla)e^N, \]

or

\[ n_e^e \frac{\partial}{\partial t}(N_e) + \nabla \cdot \left[ -n_e(\mu_e \cdot \mathbf{E}) - n_e(D_e \cdot \nabla N_e) - n_e(\nabla \cdot D_e) \right] = R_e - n_e(\mathbf{u} \cdot \nabla)N_e \]

similarly, for the electron energy density:

\[ n_e^e \frac{\partial}{\partial t}(E_n) + \nabla \cdot \left[ -n_e(\mu_e \cdot \mathbf{E}) - n_e(D_e \cdot \nabla E_n) - n_e(\nabla \cdot D_e) \right] + \mathbf{E} \cdot \Gamma_e = R_e - n_e(\mathbf{u} \cdot \nabla)E_n \]

The resulting equation system is inherently more stable than the original equation system. A useful quantity for results and analysis is the electron “temperature” (SI unit: \( \text{V} \)) which is defined as:
Source Coefficients

The source coefficients in the equations in the Electron Transport Theory section are determined by the plasma chemistry and are written using either rate or Townsend coefficients. Suppose that there are \( M \) reactions which contribute to the growth or decay of electron density and \( P \) inelastic electron-neutral collisions. In general \( P \gg M \).

In the case of rate coefficients, the electron source term is given by

\[
R_e = \sum_{j=1}^{M} x_j k_j N_n n_e
\]

where \( x_j \) is the mole fraction of the target species for reaction \( j \), \( k_j \) is the rate coefficient for reaction \( j \) (SI unit: \( m^3/s \)) and \( N_n \) is the total neutral number density (SI unit: \( 1/m^3 \)). When Townsend coefficients are used, the source term becomes

\[
R_e = \sum_{j=1}^{M} x_j \alpha_j N_n |\Gamma_e| e
\]

where \( \alpha_j \) is the Townsend coefficient for reaction \( j \) (SI unit: \( m^2 \)) and \( \Gamma_e \) is the electron flux as defined above (SI unit: \( 1/(m^2 \cdot s) \)). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

The electron energy loss is obtained by summing the collisional energy loss over all reactions:

\[
R_{e} = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta \epsilon_j
\]

where \( \Delta \epsilon_j \) is the energy loss from reaction \( j \) (SI unit: V). In the case of Townsend coefficients, the energy loss is given by

\[
R_{e} = \sum_{j=1}^{P} x_j \alpha_j N_n |\Gamma_e| e \Delta \epsilon_j
\]
The energy loss due to inelastic collisions is the most important input parameter in the Drift Diffusion interface. If this is not correctly defined, severe numerical problems result.

The rate and Townsend coefficients $k_j$ and $\alpha_j$ depend exponentially on the mean electron energy, $\bar{E}$. When a Maxwellian EEDF is assumed, the rate and Townsend coefficients can be fitted with a function of the form:

$$k_j = A e^{\beta E/\bar{E}}$$

The interface does not provide a way of calculating the rate or Townsend coefficients. The multiphysics interfaces for the most common types of reactor automatically compute the rate coefficients for each electron impact reaction based on plasma chemistry.

**Stabilization**

When the source stabilization is on, additional source terms are added to Equation 6-5 and Equation 6-6. For the electron density, the following source is added:

$$R_e = N_A \exp(-\zeta \ln(n_e))$$

where $\zeta$ is the user-defined tuning parameter. When the electron density is very low, this acts as a source term which prevents the electron density from approaching zero. As the electron density increases this term becomes exponentially smaller, eventually becoming negligible for high electron densities. A similar source is added for the electron energy density:

$$R_e = N_A \exp(-\zeta \ln(n_e))$$

**Tensor Transport Properties**

If a strong DC 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 $\mu_{dc}$ is the electron mobility in the absence of a magnetic field. The electron diffusivity, energy mobility, and energy diffusivity are then calculated using:

$$D_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{3} \right) \mu_{dc}, \quad D_e = \mu_e T_e$$

These equations are exact for a Maxwellian EEDF, a constant momentum transfer frequency and a constant kinetic pressure.

**The Wall Boundary Condition**

At the Wall, the exchange of electrons occurs through the following mechanisms:

- Loss of electrons due to a net flux of electrons from the plasma bulk to the wall.
- Loss of electrons due to the random motion of electrons within the mean free path of the wall.
- Gain of electrons due to secondary emission; a wall emits an electron with some probability when it is struck by a positive ion.
- Gain of electrons due to *thermionic emission*.

The resulting equation for the normal component of the electron flux at the wall is given by:

$$-\mathbf{n} \cdot \Gamma_e = \frac{1-r}{1+r} \left( \frac{1}{2} v_{e, \text{th}} n_e \right) - \frac{2}{1+r} (1-a) \left[ \sum_p \gamma_p \Gamma_p \cdot \mathbf{n} + \Gamma_t \cdot \mathbf{n} \right]$$

(6-8)

and for the normal component of the electron energy density:

$$-\mathbf{n} \cdot \gamma_e = \frac{1-r}{1+r} \left( \frac{5}{6} v_{e, \text{th}} n_e \right) - \frac{2}{1+r} (1-a) \left[ \sum_p \gamma_p \Gamma_p \cdot \mathbf{n} + \Gamma_t \cdot \mathbf{n} \right]$$

(6-9)

here:

- $r$ is the reflection coefficient (usually 0)
- $a$ is 1 when the electron flux is directed towards the wall and zero otherwise
- $v_{e, \text{th}}$ is the thermal velocity (SI unit: m/s)
- $n_e$ is the number density of back scattered electrons (SI unit: $1/m^3$)
- $\gamma_p$ is the secondary emission coefficient from the $p$th positive ion species
• $\Gamma_p$ is the ion flux of the $p$th positive ion species at the wall (SI unit: $1/(m^2\cdot s)$)
• $\Gamma_t$ is the thermal emission flux (SI unit: $1/(m^2\cdot s)$)
• $\varepsilon_p$ is the mean energy of the $p$th species of emitted electrons (SI unit: V)
• $\varepsilon_t$ is the mean energy of thermally emitted electrons (SI unit: V), and
• $\mathbf{n}$ is the outward normal.

The thermal velocity is defined as:

$$v_{e, \text{th}} = \frac{8k_bT_e}{\pi m_e}.$$

When the Include migration effects is activated the first term on the right-hand side of Equation 6-8 becomes:

$$\frac{1-r}{1+r}v_{e, \text{th}} n_e + n_e (\mu_e \cdot \mathbf{E}) \cdot \mathbf{n}$$

and the first term on the right-hand side of Equation 6-9 becomes:

$$\frac{1-r}{1+r}\frac{5}{6}v_{e, \text{th}} n_e + n_e (\mu_e \cdot \mathbf{E}) \cdot \mathbf{n}$$

where $\mathbf{E}$ is the electric field on the wall.

---

**The Insulation Boundary Condition**

The Insulation boundary condition simply sets the normal component of the electron and electron energy flux to zero:

$$\mathbf{n} \cdot \Gamma_e = 0 \quad \text{and} \quad \mathbf{n} \cdot \Gamma_{\varepsilon} = 0$$

---

**The Electron Density and Energy Boundary Condition**

The Electron Density and Energy boundary condition fixes the electron density to a specific number density or the mean electron energy to a specific energy. This boundary condition should, in general, be avoided in favor of the Wall boundary condition.

$$n_e = n_{ew} \quad \text{and} \quad \bar{\varepsilon} = \bar{\varepsilon}_0$$
Due to the fact that the log of the electron density is solved for, specifying an electron density of zero is not allowed.

Reference for the Drift Diffusion Interface


The Heavy Species Transport Interface

This chapter describes the Heavy Species Transport interface, which is a mass balance interface for all non-electron species. This includes charged, neutral, and electronically excited species. The Heavy Species Transport interface, found under the Plasma branch when adding a physics interface, also makes it possible to add electron impact reactions, chemical reactions, surface reactions, and species via the Model Builder.

In this chapter:

- The Heavy Species Transport Interface
- Theory for the Heavy Species Transport Interface
The Heavy Species Transport Interface

The Heavy Species Transport (hs) interface ( ), found under the Plasma branch ( ), when adding a physics interface, adds electron impact reactions, gas phase reactions, and species and surface reactions to plasma models. The most convenient way to do this is to load a set of collision cross sections from a file in the Cross Section Import section from the Heavy Species Transport settings window.

INTERFACE IDENTIFIER

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

The default identifier (for the first interface in the model) is hs.

DOMAIN SELECTION

The default setting is to include All domains in the model to define the dependent variables and the equations. To choose specific domains, select Manual from the Selection list.

TRANSPORT SETTINGS

Select a Diffusion model—Mixture-averaged (the default) or Fick’s law. When using the Mixture-averaged model, the binary diffusion coefficients are automatically computed based on the data specified for each species.

Select an Equation formulation—Log (the default) to solve the equations in logarithmic form or Linear to solve equations in the original form. Log solves for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve.

The Migration in electric field check box is selected by default. The Migration term is part of the total mass flux vector. Select the check boxes for other transport mechanisms to Include—Convection, Calculate thermodynamic properties, Full expression.
for diffusivity, or Compute tensor ion transport properties. The selection changes the number of Model Inputs requiring values on the Diffusion, Migration settings window. Note the following:

- **Convection** of heavy species present in a plasma can often be neglected due to the low operating pressure.
- If **Calculate thermodynamic properties** is selected, select the thermodynamic properties of each reaction and species are computed automatically based on the thermodynamic properties of each species.
- If **Full expression for diffusivity** is selected, it computes a more accurate expression for the binary diffusion coefficients. Often the additional correction terms (the collision term, \( \Omega_D \) given by Equation 7-17 and used in Equation 7-16) are negligible in which case the expressions are much simpler and the time taken to assemble the Jacobian matrix is reduced.
- If the **Compute tensor ion transport properties** option is selected, the tensor form of the ion transport properties when a static magnetic field is present are computed. This option only needs to be activated when a strong DC magnetic field exists and the operating pressure is very low (on the order of millitorr). When this option is activated an expression must be provided for the magnetic flux density which would typically be computed by another physics interface. This is set in the Convection, Migration, Diffusion feature.

**ELECTRON ENERGY DISTRIBUTION FUNCTION SETTINGS**

If cross-section data is used to define source coefficients in the model then an electron energy distribution function (EEDF) needs to be selected. These options are available.

- **Maxwellian.** This option assumes a Maxwellian EEDF which takes the form:

\[f(\epsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\epsilon \beta_2 / \varphi\right)\]

where

\[\beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1}\]

For more information on the electron energy distribution function (EEDF), see the Theory for the Boltzmann Equation, Two-Term Approximation Interface.
where $\varphi$ is the mean electron energy (eV), $\varepsilon$ is the electron energy (eV) and $\Gamma$ is the incomplete gamma function.

- **Druyvesteyn.** This option assumes a Druyvesteyn EEDF which takes the form:

$$f(\varepsilon) = 2\varphi^{-3/2}\beta_1 \exp\left(-\frac{\varepsilon \beta_2}{\varphi}\right)$$

where

$$\beta_1 = \Gamma(5/4)^{3/2}\Gamma(3/4)^{5/2}, \beta_2 = \Gamma(5/4)\Gamma(3/4)^{-1}$$

- **Generalized.** Use this option for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. If this option is selected, specify a power law. This number must be between 1 and 2. Mathematically, the EEDF takes the form:

$$f(\varepsilon) = g\varphi^{-3/2}\beta_1 \exp\left(-\frac{\varepsilon \beta_2}{\varphi}\right)^g$$

where

$$\beta_1 = \Gamma(5/2g)^{3/2}\Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g)\Gamma(3/2g)^{-1}, 1 \leq g \leq 2$$

- **Function.** If a two dimensional interpolation function has been added to the model, it can be used for the EEDF. In this case, the $x$-data should be the electron energy (eV) and the $y$-data should be the mean electron energy (eV).

The two-dimensional interpolation function can be computed using a parametric sweep in *The Boltzmann Equation, Two-Term Approximation Interface*. This allows for modeling of discharges where the EEDF is far from Maxwellian.

In all these cases the rate constants in the model are automatically computed based on the selected EEDF using the formula:

$$k_T = \gamma \int_0^{\infty} \varepsilon \sigma_0(\varepsilon)f(\varepsilon) d\varepsilon$$  \hspace{1cm} (7-1)

The rate coefficients when computed using cross section data are a highly nonlinear function of the mean electron energy. COMSOL Multiphysics automatically computes the integral in Equation 7-1 and makes the result available for evaluation of the rate coefficient. The variation of the rate coefficient for any particular model can be plotted.
using <interface identifier>.kf_<reaction number>. For example, for reaction number 3 in a heavy species interface, with identifier hs, the rate coefficient would be plotted using hs.kf_3.

**CHEMKIN**
Import thermodynamic and transport properties for the reacting species into the model.

**STABILIZATION**
If the **Equation formulation** is set to Log then the solver can run into difficulties when the species mass fractions approach zero. The **Reaction source stabilization** check box (selected by default) adds an additional source term to the rate expression for each species. In the t edit field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

**DISCRETIZATION**
To display this section, click the **Show** button ( ) and select **Discretization**. Select an **Element order**—Linear (the default), Quadratic, Cubic, or Quartic. Specify the **Value type** when using splitting of complex variables—Real or Complex (the default).

- Stabilization
- Show More Physics Options
- Domain, Boundary, and Pair Nodes for the Heavy Species Transport Interface
- Theory for the Heavy Species Transport Interface
- Interpolation in the COMSOL Multiphysics Reference Manual

Surface Chemistry Tutorial: model library path
Plasma_Module/Chemical_Vapor_Deposition/surface_chemistry_tutorial
Domain, Boundary, and Pair Nodes for the Heavy Species Transport Interface

The Heavy Species Transport Interface has these domain, boundary, 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. However, to add subnodes, right-click the parent node.

The boundary conditions are available for both charged and neutral species. Surface reactions can be added to the model—COMSOL Multiphysics then automatically generates the appropriate expressions for the fluxes for each species on the boundaries. Boundary conditions do not need to be applied for a species that comes from the mass constraint condition.

- Cross Section Import
- Diffusion and Migration
- Electron Impact Reaction
- Flux
- Inlet
- Outflow
- Reaction
- Species
- Surface Reaction
- Surface Species
- Symmetry

Due to the overwhelming number of species that can exist in a plasma, the Flux, Inlet, Outflow, and Symmetry boundary condition subfeatures can be assigned by right-clicking the Species node in the Model Builder. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.
In the COMSOL Multiphysics Reference Manual:

- Continuity on Interior Boundaries
- Identity and Contact Pairs

Cross Section Import

The Cross Section Import node allows you to import collision cross section data into the model. The cross section data must be in a specific format. Browse to a file containing a set of collision cross sections.

The file must follow the format documented in Importing Collision Cross-Section Data.

Diffusion and Migration

The Diffusion and Migration node sets up the model inputs for the interface. Choose how to define the density of the gas mixture.

The node name changes to Diffusion or Convection, Diffusion, and Migration based on the check boxes selected in the Transport Settings section.

DOMAIN SELECTION

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

MODEL INPUTS

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs display here. Initially, this section is empty. The input depends on which Transport Settings are selected on The Heavy Species Transport Interface.

- Enter a Temperature $T$ (SI unit: K) for the gas mixture used to compute the gas density and species transport properties.
• Enter an **Absolute pressure** $p$ (SI unit: Pa) to compute the gas density and the binary diffusion coefficients.

• When the default **Migration in electric field** check box is selected, enter an **Electric potential** $V$ (SI unit: V). This is used to compute the electric field that results in migration of any charged species.

• If the **Convection** check box is selected, enter coordinates for the **Velocity field** $\mu$ (SI unit: m/s).

• If the **Compute tensor electron transport properties** check box is selected, enter coordinates for the **Magnetic flux density** $B$ (SI unit: T). This usually comes from a magnetostatic model, and is used to compute anisotropic transport properties for electrons.

**Density**

Select an option from the **Mixture density** list—**Ideal gas** (the default) or **User defined**. If **User defined** is selected, enter a value for $\rho$ (SI unit: kg/m$^3$).

If **Ideal gas** is selected, it computes the expression for the gas density automatically using the ideal gas law, based on the composition of the mixture. The density is a function of the mean molecular weight

$$\rho = \frac{p_A M_n}{R T}$$

where $p_A$ is the absolute pressure, $T$ is the temperature, $R$ is the universal gas constant, and $M_n$ is the mean molar mass given by

$$\frac{1}{M_n} = \sum_{k=1}^{Q} \frac{w_k}{M_k}$$

**Electron Impact Reaction**

The **Electron Impact Reaction** node ($\star_e$) sets up the reaction rate for a reaction involving an electron and a target species.

**Domain Selection**

From the **Selection** list, choose the domains to define.
REACTION FORMULA

Enter chemical reaction formulas in the Formula edit field. The interface examines the species taking part in the reaction and automatically adds the associated Species features to the Model Builder.

Electron impact reactions are always assumed to be irreversible. However, the reverse reaction is automatically created if it is specified that a detailed balance should be constructed in the cross section data file. See Importing Collision Cross-Section Data.

Entering a Formula

The letter “e” is reserved to represent an electron. Therefore if a formula such as e+Ar=>e+Ar+ is entered, the species e is automatically assigned as an electron.

Valid species names consist of a case-sensitive combination of letters, numbers, and “+” or “-” signs. With the exception of the “+” and “-” signs, which are used for ions, special characters are not allowed as species names or part of species names (for example, (), [], *, #, and _). In addition, the first character in a species name must be a letter to avoid confusion with the stoichiometric coefficients in the reaction formula. Ions are labeled with one plus or minus sign per species charge added directly after the species name. For example, O++ represents an oxygen atom with a twofold positive charge; O2+ represents molecular oxygen with a single positive charge; and 2O+ represents two oxygen atoms, each with a single positive charge. This automatically fills in the charge of the species ion the Charge edit field in the associated Species node.

COLLISION TYPE

This section is available when a valid formula for the electron impact reaction is entered.

Select a Collision type—Elastic (the default), Excitation, Attachment, or Ionization.

- If Elastic is selected, enter a value for the Electron mass ratio \( m_e \) (dimensionless) (the ratio of the mass of the electron to the target species).
• Select **Excitation** for excitation reactions where the collision is inelastic. Enter the *Energy loss* $\Delta e$ (SI unit: V) for the reaction. This is also known as threshold energy for the reaction. Select this option for electronic excitation, vibrational and rotational excitation, and superelastic collisions. For superelastic collisions, the activation energy is negative.

• Select **Attachment** for collisions which result in the electron attaching to the target species, forming a negative ion. No user input is required.

• Select **Ionization** for electron impact reactions which result in secondary electrons being formed. Enter the *Energy loss* $\Delta e$ (SI unit: V) for the reaction. This is also known as threshold energy for the reaction.

**COLLISION**

<table>
<thead>
<tr>
<th></th>
<th>This section is available when a valid formula for the electron impact reaction is entered.</th>
</tr>
</thead>
</table>

Specify how to specify the reaction rate constant. There are these options:

• **Cross section data.** If this option is selected, enter cross section data directly into a table for the electron impact reaction.

• **Arrhenius parameters.** With this option, use Arrhenius coefficients to specify the reactions dependence on the electron “temperature,” $T_e$.

• **Rate constant.** Use this option to specify an arbitrary expression for the rate constant. This can be a numeric value or a complicated function of the electron “temperature,” gas temperature or any other expression. This is the default option for specifying the reaction.

• **Use lookup table.** Use this option to either enter or load in a lookup table of the source coefficient versus mean electron energy.

**CROSS SECTION DATA**

<table>
<thead>
<tr>
<th></th>
<th>This section is available when a valid formula is entered for the electron impact reaction and the Specify reaction using option is set to Cross section data in the Collision section.</th>
</tr>
</thead>
</table>

By default the electron energy distribution function is taken from the physics interface property. It can be changed to **Maxwellian**, **Druyvesteyn**, or **Generalized**. In this case, the
selected distribution function is only used in the current electron impact reaction. The Electron energy in the Collision cross section data table should have units of electronvolts (eV). The units of the Collision cross section data has units of m².

If a set of collision cross sections are loaded from a file with the Cross Section Import node, the software automatically generates the electron impact collisions and enters the cross section data into the Collision cross section data table.

Electron Energy Distribution Function Settings

ARRHENIUS PARAMETERS
If Arrhenius parameters is selected to specify the reaction then COMSOL Multiphysics automatically generates an expression of the form

\[ k_f = A_f T_e^{n_f} \exp(-E_f / T_e) \]

for the rate constant. Here, \( A_f \) is the forward frequency factor, \( n_f \) is the electron temperature exponent and \( E_f \) is the activation energy (eV). The quantity \( T_e \) is the electron “temperature” (eV) which is defined as

\[ T_e = \frac{2 \tilde{e}}{3} \]

where \( \tilde{e} \) is the mean electron energy.

KINETIC EXPRESSIONS
If the Specify reaction using option is set to Rate constant then enter in an expression for the reaction forward rate constant in the Forward rate constant edit field. The units of the rate constant depend on the order of the reaction.

<table>
<thead>
<tr>
<th>ORDER</th>
<th>EXAMPLE</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O₂ → 2O</td>
<td>1/s</td>
</tr>
<tr>
<td>2</td>
<td>O + O₂ → O₃</td>
<td>m³/(s·mol)</td>
</tr>
<tr>
<td>3</td>
<td>3O → O₂ + O</td>
<td>m⁶/(s·mol²)</td>
</tr>
</tbody>
</table>
**Source Coefficient Data**

If the **Specify reaction using** option is set to **Use lookup table** then the **Source coefficient** data section appears. Choose between **Rate coefficients** and **Townsend coefficients** to specify the source coefficients. If **Rate coefficients** is selected then either enter in the lookup table or load in from file a table of mean electron energy (eV) versus rate coefficient (SI unit: m³/s). If **Townsend coefficients** is selected, then enter in or load data from file a table of mean electron energy (eV) versus Townsend coefficient (SI unit: m²).

**Reaction**

Use the **Reaction** node ( ) to enter reversible or irreversible reactions which don’t involve electrons, for example for gas phase reactions. Enter the **Formula** for the reaction into the field and then fill in the appropriate information about the reaction.

**Domain Selection**

From the **Selection** list, choose the domains to define. COMSOL Multiphysics automatically ensures that the **Reaction** selection is the same as the **Diffusion and Migration** selection.

**Reaction Formula**

See the Reaction Formula settings for the **Electron Impact Reaction** node.

**Arrhenius Parameters**

This section is available when a valid formula for the reaction is entered.

Choose whether or not to use Arrhenius expressions to compute the reaction forward and reverse rate constants using:

\[ k = A T^n \exp\left(-\frac{E}{R_g T}\right) \]
To activate the Arrhenius Parameters section and make the kinetic expressions use these parameters, select the Use Arrhenius expressions check box. In the Arrhenius Parameters section, $A$ denotes the frequency factor, $n$ the temperature exponent, $E$ the activation energy (SI unit: $J/mol$), and $R_g$ the gas constant, $8.314\ J/(mol\cdot K)$. The pre-exponential factor, including the frequency factor $A$ and the temperature factor $T^n$, is given the units $(m^3/mol)^{α-\frac{1}{2}}/s$, where $α$ is the order of the reaction (with respect to the concentrations). Edit fields are available for each of the Arrhenius parameters in the equation above.

**Kinetic Expressions**

Modify the default expressions for the rate constant. This field is only available if the Use Arrhenius check box is cleared. The units of the rate constant depend on the order of the reaction.

**Table 7.2: SI Units for the Rate Constant for Different Reaction Orders**

<table>
<thead>
<tr>
<th>ORDER</th>
<th>EXAMPLE</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O₂⇒O₂</td>
<td>1/s</td>
</tr>
<tr>
<td>2</td>
<td>O+O₂⇒O₃</td>
<td>m³/(s·mol)</td>
</tr>
<tr>
<td>3</td>
<td>3O⇒O₂+O</td>
<td>m⁶/(s·mol²)</td>
</tr>
</tbody>
</table>

**Species**

Use the Species node ( ) to add additional species to the model even if they do not participate in any reactions.

Due to the overwhelming number of species that can exist in a plasma, the Flux, Inlet, Outflow, and Symmetry boundary condition subfeatures can be assigned by right-clicking the Species node in the Model Builder. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

Species are automatically added to the model when reactions are added.
**DOMAIN SELECTION**

From the Selection list, choose the domains to define. COMSOL Multiphysics automatically ensures that the Species selection is the same as the Diffusion and Migration selection.

**SPECIES FORMULA**

Species Name

Enter basic information about the name and nature of the species. When a new species is created, the Species name field is editable. A valid name for the species must be entered, for example, o2, Ar, Ar+. After the species name has been entered the edit field cannot be edited (as long as a valid species name is entered).

Species Type

The Species type is either Neutral, Ion, or Electron.

- Enter “e” to automatically create a species as an Electron. The Species node is renamed to include the name entered in the Species type field. Also enter the Electron Parameters.
- Enter a neutral species, for example, o2 to automatically create a species as Neutral.
- Enter a charged species, for example, Ar+ or o2- to automatically create a species as an Ion. The Species node is renamed to include the name entered in the Species type field. When the species created is an Ion, also select the Initial value from electroneutrality constraint check box to indicate that the initial mass fraction of this species is automatically computed based on the initial electron density specified in the electron species properties. This ensures that the solver can find consistent initial conditions when starting because the plasma is initially electrically neutral. Also enter the General Parameters described in the next section.
- If Neutral is selected as the Species type, enter the General Parameters described in the next section.

When Neutral is selected, also select the From mass constraint check box to indicate which species should be used as the mass constraint and therefore not solved for. This is typically the species with the highest mass fraction. It should not be a species whose mass fraction is a very small value (as is the case with ionic species).
GENERAL PARAMETERS

This section is available when the Species type under Species Formula selected is Ion or Neutral. Enter the physical properties of the species. Enter the following properties:

- **Preset species data.** The default value is User defined which means that the transport properties are computed from the values given in the edit fields below. There is preset transport data available for the most common gases encountered in plasma processing. Selecting one of these gases fills in the correct values for the species transport properties automatically.

- **Molecular weight** $M_w$ (SI unit: kg/mol) of the species. The default value for the molecular weight is 0.032. The molecular weight must be a nonzero number.

- **Charge** $z$ (dimensionless) number of the species. The charge number is automatically computed from the formula specified via either a reaction or by manually creating a species.

- **Potential characteristic length** $\sigma$ (SI unit: m). The potential characteristic length is used to compute the binary diffusion coefficients used in the Mixture-Averaged transport setting.

- **Potential energy minimum** $e/k_B$ (SI unit: m). This is used to compute the binary diffusion coefficients.

- **Dipole moment** $\mu_D$ (SI unit: Cm). If the dipole moment is known, enter its value and obtain a more accurate expression for the binary diffusion coefficients.

- **Thermal diffusion coefficient** $D_T$ (SI unit: $m^2/s$). If thermophoretic effects are important in the model then enter a value for the thermal diffusion coefficient.

- **If Neutral is selected as the Species type, enter an Initial mole fraction** $x_0$ (dimensionless). Set the initial mole fraction of the selected species in the gas mixture. If the From mass constraint check box is selected, this field is not available.

- **If Ion is selected as the Species type, enter an Initial number density** $n_0$ (dimensionless) to set the initial number density of the selected species in the gas mixture. If the Initial condition from electroneutrality constraint check box is selected, this field is not available.

- **Diffusion coefficient** $D_f$ (SI unit: $m^2/s$). If the Diffusion model property is set to Fick’s law then the diffusion coefficient isn’t computed automatically from the transport properties, its value is taken from this edit field.
ELECTRON PARAMETERS
This section is available when the Species type under Species Formula selected is Electron. Enter the physical properties of the species. Enter the following properties:

• Electron density \( n_e \) (SI unit: \( 1/m^3 \)).
• Mean electron energy \( e \) (SI unit: V).
• Initial electron density \( n_{e,0} \) (SI unit: \( 1/m^3 \)).

SPECIES THERMODYNAMIC PARAMETERS
This section is available if the Calculate thermodynamic properties is check box is selected under Transport Settings on the Heavy Species Transport interface.

Enter thermodynamic properties for the species using the NASA polynomial format. Any coefficients for the thermodynamic polynomials are entered into the \( a_{low,k} \) fields and apply to the temperatures in the range \( T_{inc/lower} \) to \( T_{inc/midpoint} \); coefficients entered into the \( a_{hi,k} \) fields apply to temperatures in the range \( T_{inc/midpoint} \) to \( T_{inc/upper} \) range.

• Enter the Lower temperature limit \( T_{lo} \), Middle temperature limit \( T_{mid} \), and Upper temperature limit \( T_{hi} \). The defaults are 300 K, 1000 K, and 5000 K respectively.
• Enter the Polynomial coefficients \( a_{low,k} \) and \( a_{hi,k} \).
• Enter an Additional enthalpy contribution \( \Delta h \) (SI unit: V) as required.

MOBILITY AND DIFFUSIVITY EXPRESSIONS
This section is available when the Species type under Species Formula selected is Ion. The default specification is to compute the diffusivity and mobility from the binary diffusion coefficients and Einstein’s relation.

Select a Specification—Compute mobility and diffusivity or Specify mobility, compute diffusivity.

The Mobility is computed using Einstein’s relation by default. If Mixture averaged is selected as the Diffusion model under Transport Settings on the Heavy Species Transport interface, then the mobility is computed using:

\[
\mu = \frac{D_m q}{k_B T}
\]

and if the Fick’s law property is selected, then the mobility is defined as:
\[
\mu = \frac{Dq}{k_B T}
\]

Select an Ion temperature—Use gas temperature or Specify ion temperature. If Specify ion temperature is selected, enter an Ion temperature \( T_{\text{ion}} \) (SI unit: K). The default is 300 K.

**Mobility Specification**

This section is available if Specify mobility, compute diffusivity is selected under Mobility and Diffusivity Expressions.

Select an option from the Specify using list—Constant value or Lookup table.

- If Constant value is selected, enter a value or expression for the Mobility \( u_m \) (SI unit: m²/Vs). This can be a function of any of the variables in the model.
- If Lookup table is selected, the mobility is then a function of the electric field. Select an option from the Mobility a function of list—Electric field or Reduced electric field. Enter values into the table or click the Load from file button ( ) to import data from a text file. The file must contain the two columns of data, the Electric field (SI unit: V/m) or the Reduced electric field (SI unit: Vm²) as the x-data and the ion mobility (SI unit: m²/(V-s)) or reduced ion mobility (SI unit: 1/(m-V-s)) as the y-data.

Select the Use local field approximation for ion temperature check box to automatically compute the ion temperature using the local field approximation. The local field approximation can be useful for high pressure discharges where the electric field is very high, as is the case for dielectric barrier discharges.

**Surface Reaction**

The Surface Reaction node ( ) sets up reactions involving gas phase, surface, and bulk species on surfaces. Surface reactions play an important role in the overall characteristics of a discharge. This typically involves first order reactions on surfaces where excited or ionic species transition back to their ground state.

**Boundary Selection**

From the Selection list, choose the boundaries to define.
PAIR SELECTION
If this node is selected from the Pairs menu, choose the pair to define. An identity pair has to be created first. Ctrl-click to deselect.

REACTION FORMULA
The first thing to input after creating a new reaction is the Reaction Formula. The reaction can only be irreversible. Valid species names consist of a case-sensitive combination of letters, numbers, and “+” or “-” signs. With the exception of the “+” and “-” signs, which are used for ions, special characters are not allowed as species names or part of species names (for example, [], *, #, and _). In addition, the first character in a species name must be a letter to avoid confusion with the stoichiometric coefficients in the reaction formula. Ions are labeled with one plus or minus sign per species charge added directly after the species name.

For surface reactions, use the notation (s) to denote surface species or (b) to denote bulk species. This is bulk surface species, not to be confused with gas phase species. The species is then called name _surf or name_bulk depending on the species type. For example, using Si(s) in the reaction formula creates a surface species with the name Si_surf and Si(b) creates a surface species with the name Si_bulk.

Under Specify reaction using select whether to specify the surface reaction using Sticking coefficient or Rate coefficient. Sticking coefficients are typically easy to estimate intuitively and must be between 0 and 1. Rate coefficients require specification of a rate constant, which can be obtained in the appropriate literature.

Under Motz-Wise correction select whether to include this correction in the expression for the rate constant. This option is only available when the reaction is specified using sticking coefficients. When the Motz-Wise correction is set to On, Equation 7-19 is used to compute the rate constant. When set to Off, Equation 7-20 is used.

Only irreversible surface reactions are supported.

ARRHENIUS PARAMETERS
This section is available when a valid formula for the surface reaction is entered.
Choose whether or not to use Arrhenius expressions to compute the sticking coefficients. When this option is activated the expression for the sticking coefficient is automatically computed using:

$$\gamma = aT^b \exp\left(\frac{e}{R_g T}\right)$$

where $a$ is the frequency factor, $b$ is the temperature exponent, and $e$ is the activation energy (SI unit: J/mol).

**Kinetic Expressions**

Enter the Forward sticking coefficient for the surface reaction. The option is available if the Use Arrhenius expressions check box is not selected.

**Surface Species**

The Surface Species ( ) node adds detailed surface chemistry to the model. The species can either be surface (for example, Si(s)) or bulk species (for example, Si(b)). This is usually generated by default when a formula for a surface reaction is entered.

**Species Formula**

Enter a formula for the surface species. The symbols (s) and (b) are reserved to denote surface species or bulk species, respectively. So, to create a silicon surface species simply type $\text{Si}(s)$. To create a silicon bulk species type $\text{Si}(b)$. COMSOL Multiphysics automatically renames the species to a valid name, for example $\text{Si}_{\text{surf}}$ or $\text{Si}_{\text{bulk}}$.

**General Parameters**

Enter the molecular weight (SI unit: kg/mol) of the surface or bulk species. The default value is User defined which means that the surface species properties are computed from the values given in the edit fields below. There is preset transport data available some of the typical surface species encountered in plasma processing. Selecting one of these fills in the correct values for the molecular weight and thermodynamic properties automatically.

**Surface Species Parameters**

If the species is a surface species then this section is available.

- Enter the Site occupancy number $\sigma$ (dimensionless) of the species. The default value is 1. This accounts for the fact that larger molecules can occupy more than one active site on a surface.
• Enter the **Initial density of surface sites** $\Gamma_{n,0}$ (SI unit: mol/m$^2$) of the species. The default value is 1.95E-5. This surface site concentration remains constant, with this initial value if every surface species has the same site occupancy number.

• The **Initial site fraction** $Z_{k,0}$ (dimensionless) is the initial fraction of the total sites which is occupied by the species. This must be a number between 0 and 1.

**BULK SPECIES PARAMETERS**

If the species is a bulk species then enter the density (SI unit: kg/m$^3$). The default value is 2329 kg/m$^3$ corresponding to the density of silicon.

---

**Flux**

Due to the overwhelming number of species which can exist in a plasma, the Flux boundary condition can be assigned by right-clicking the Species node in the Model Builder. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The Flux subnode prescribes the mass flux of the selected species on selected boundaries. A user-defined normal flux is available via the equation:

$$-\mathbf{n} \cdot \rho w_k (\mathbf{V}_k + \mathbf{u}) = \Gamma_k$$

---

**Inlet**

Due to the overwhelming number of species which can exist in a plasma, the Inlet boundary condition can be assigned by right-clicking the Species node in the Model Builder. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The Inlet subnode adds a boundary condition for an inflow boundary, where a condition for all species is specified. The condition can be specified using these quantities:

• The mass fraction: $\omega = \omega_0$,
• The mole fraction: $x = x_0$,
• The molar concentration (SI unit: mol/m$^3$) $c = c_0$,
• The number density, which describes the number of particles per volume (SI unit: 1/m$^3$): $n = n_0$.
A concentration quantity other than the mass fractions can only be used when all species are defined, as in the Inlet condition. The other quantities are composition dependent and therefore unambiguous only when all species are defined.

**BOUNDARY SELECTION**
From the Selection list, choose the boundaries to define.

**INLET**
Select the type of input from the Mixture specification list:

- Select **Mass fraction** (the default) to enter mass fractions ($\omega_0, \omega_1$, for example).
- Select **Mole fraction** to enter mole fractions ($x_0, x_1$, for example).
- Select **Molar concentration** to enter molar concentrations ($c_0, c_1$, for example).
- Select **Number density** to enter number densities ($n_0, n_1$, for example).

Type the value or expression in the edit fields for each species except the one computed from the mass constraint.

---

**Outflow**
Due to the overwhelming number of species that can exist in a plasma, the Outflow boundary condition can be assigned by right-clicking the Species node in the Model Builder. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The Outflow subnode is used on boundaries where the species mass is to be transported out of the model domain.

If an imaginary slice is drawn through the cross section of a geometry, then there is no net flux across the slice due to diffusion, since diffusion corresponds to random motion of the atoms and molecules. There can, however, be a net flux due to convection, migration or thermophoresis, but outlet boundary conditions for temperature and electric field also impose zero gradient. An appropriate “open” boundary condition is

---

When using the Logarithmic form of the equations, setting a zero value for any of the options listed above results in an error when attempting to solve. To avoid the solver taking $\log(0)$ a positive, nonzero value must be entered.
to set the normal component of the diffusive flux to zero, which implies that diffusive transport of flux across the imaginary slice is zero. The boundary condition becomes:

\[-n \cdot j_k = 0\]

which assumes that all mass passing through the boundary is due to convection.

**Symmetry**

Due to the overwhelming number of species which can exist in a plasma, the **Symmetry** boundary condition can be assigned by right-clicking the **Species** node in the **Model Builder**. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The **Symmetry** subnode is used on all boundaries where the selected species mass fraction is symmetric. This is identical to the **No Flux** boundary condition. The symmetry boundary imposes a zero flux boundary condition.
Theory for the Heavy Species Transport Interface

The Heavy Species Transport Interface theory is described in this section:

- About the Transport Equations
- Scaling
- Multicomponent Diffusion Equations
- Stabilization
- Additional Quantities of Interest
- Surface Reactions
- Auxiliary Relations
- Flux Matching
- Source Coefficients
- About Surface Species
- Thermodynamic Properties
- Limitations of the Heavy Species Transport Equations
- Species Transport Properties
- References for the Heavy Species Transport Interface
- Mixture Transport Properties

About the Transport Equations

There are a number of different formulations available for modeling mass transport, ranging from a simple reaction, convection, diffusion equation to the Maxwell-Stefan (sometimes called Stefan-Maxwell) equations. The Maxwell-Stefan equations are the only formulation that conserves the total mass in the system and also satisfies a number of auxiliary constraints. The main drawback of the Maxwell-Stefan equations is the amount of computational resources needed to solve them. In many situations, simplified forms of the Maxwell Stefan equations can be applied, which do not rigorously satisfy the laws of multicomponent diffusion but are much easier to implement and consume less computational resources.

Neutral and excited species in a plasma require a suitable transport equation. Typically the concentration of excited species is very low and they can be considered dilute. This is true with atomic gases, where the concentration of ions and electronically excited species is much lower than the concentration of the ground state atoms. Molecular gases can dissociate into stable neutral fragments via electron impact dissociation. These fragments can have a long lifetime and accumulate inside a reactor. In this case, the dilute approximation is no longer valid and a more rigorous description of the mass...
transport is necessary. Conservation of mass dictates that the sum of the mass fractions of all the species must equal one. The most accurate technique is to solve the Maxwell-Stefan equations which correctly take into account diffusive transport due to mole fraction, pressure and temperature gradients. The Maxwell-Stefan equations quickly become computationally very expensive when the number of species becomes large (>6). In a plasma, there might be 20+ neutral and excited species, so solving the full Maxwell-Stefan equations is not practical.

The Heavy Species interface provides two different Diffusion models to choose from, Mixture averaged and Fick’s law. The Mixture averaged option fulfills all the criteria for mass conservation. It is much less computationally expensive to solve than the full Maxwell-Stefan equations, which are not available in the Heavy Species interface. The Fick’s law option uses an even simpler diffusion model, which is less accurate than the Mixture averaged model, but is computationally less expensive.

**Multicomponent Diffusion Equations**

Suppose a reacting flow consists of \( k = 1, \ldots, Q \) species and \( j = 1, \ldots, N \) reactions. The equation for the first \( Q - 1 \) species is given by

\[
p \frac{\partial}{\partial t}(w_k) + \rho (\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k \tag{7-2}
\]

where:

- \( \mathbf{j}_k \) is the diffusive flux vector
- \( R_k \) is the rate expression for species \( k \) (SI unit: kg/(m\(^3\)·s))
- \( \mathbf{u} \) is the mass averaged fluid velocity vector (SI unit: m/s)
- \( \rho \) denotes the density of the mixture (SI unit: kg/m\(^3\)), and
- \( w_k \) is the mass fraction of the \( k \)th species (1).

The diffusive flux vector is defined as:

\[
\mathbf{j}_k = \rho w_k \mathbf{V}_k
\]

where and \( \mathbf{V}_k \) is the multicomponent diffusion velocity for species \( k \). The definition of \( \mathbf{V}_k \) depends on the option chosen for the Diffusion Model property. If Mixture Averaged is chosen then:

\[
\mathbf{V}_k = \frac{\nabla w_k}{w_k} + \frac{\nabla M_n}{M_n} + \frac{D_k}{\rho w_k} \frac{T}{T} + \frac{T}{T} - \frac{T}{T} - z_k \mu_{k,m} \mathbf{E}
\]
where

- $D_{k,m}$ is the mixture averaged diffusion coefficient (SI unit: m\(^2\)/s)
- $M_n$ is the mean molar mass of the mixture (SI unit: kg/mol)
- $T$ is the gas temperature (SI unit: K)
- $D^T_k$ is the thermal diffusion coefficient for species $k$ (SI unit: kg/(m·s))
- $z_k$ is the charge number for species $k$ (SI unit: dimensionless)
- $\mu_{k,m}$ is the mixture averaged mobility for species $k$ (SI unit: m\(^2\)/(V·s))
- $E$ is the electric field (SI unit: V/m)

The mixture averaged diffusion coefficient, $D_{k,m}$ for species $k$ is defined as:

$$D_{k,m} = \frac{1}{Q} \frac{1 - w_k}{\sum_{j \neq k} x_j/D_{kj}}$$  \hspace{1cm} (7-3)

The mean molar mass, $M_n$ is computed using the sum of the mass fractions and molecular weights of all species:

$$\frac{1}{M_n} = \sum_{k=1}^{Q} \frac{w_k}{M_k} .$$

The mole fraction for species $k$, which is required in Equation 7-3 can be computed from the mass fraction of species $k$ and the mean molar mass:

$$x_k = \frac{w_k}{M_k} M_n .$$

The quantity, $D_{kj}$ is the binary diffusion coefficient between species $k$ and $j$ and are rather complicated functions of the physical properties of the species. They are defined later, in Equation 7-12.

By default, the mixture averaged mobility, $\mu_{k,m}$ is computed using Einstein’s relation:

$$\mu_{k,m} = \frac{q D_{k,m}}{k_B T}$$

where $q$ is the unit charge (SI unit: s A) and $k_B$ is Boltzmann’s constant (SI unit: J/K).

For ions, it is possible to specify an arbitrary expression for the mobility in the Mobility
and Diffusivity Expressions and Mobility Specification sections. One option is to use something called the Local Field Approximation. In this case, the mobility is specified via a lookup table, the local field approximation can be used to compute the ion temperature and thus the diffusivity through Einstein’s relation, see Ref. 7. The ion temperature is computed using:

\[ T_i = T + \left( \frac{m_k + m_n}{5m_k + 3m_n} \right) \frac{m_p}{k_b} (\mu \cdot E) \cdot (\mu \cdot E) \]

where \( M_k \) is the ion mass (SI unit: kg), \( T \) is the background gas temperature (SI unit: K), \( M_n \) is the mean mass of the mixture (SI unit: kg), and \( E \) is the electric field (SI unit: V/m).

If the Diffusion Model is changed to Fick’s law then the diffusion coefficient must be given as an input for each species. In this case, the diffusion velocity is defined as:

\[ V_k = D_{k,f} \frac{\nabla w_k}{w_k} + D_{k,f} \frac{\nabla M_n}{M_n} + \frac{D_k}{\rho w_k} \frac{T}{T} \nabla - z_k \nu_{k,f} E \]

where \( D_{k,f} \) is the user-defined diffusion coefficient for species \( k \). The mobility for species \( k \) is then given by:

\[ \nu_{k,f} = \frac{q D_{k,f}}{k_B T} \]

This approach is much less computationally expensive than the Mixture averaged model since the diffusion coefficients are not computed from the complicated expression in Equation 7-3.

**Additional Quantities of Interest**

The Heavy Species interface also defines a number of additional variables for quantities which are typically of interest during results processing. The number density of species \( k \) is given by:

\[ n_k = \left( \frac{p}{k_B T} \right) \nu_k \]

where \( p \) (SI unit: Pa) is the absolute pressure of the fluid. The molar concentration of species \( k \) is given by
The density of the mixture is given by the ideal gas law by default:

\[ \rho = \frac{pM_n}{RT} \]

where \( R \) is the universal gas constant (SI unit: J/(mol K)).

A useful quantity in systems where large thermal gradients exist (that is, chemical vapor deposition processes) is the thermal drift velocity (SI unit: m/s), which is defined as

\[ \mathbf{v}^T = \frac{D^*_k}{\rho w_k} \mathbf{\nabla} \ln T \]

**Auxiliary Relations**

Only \( Q - 1 \) of the Maxwell-Stefan equations are independent and so a closure law is required. One way of ensuring a unique solution is the use the fact that the sum of the diffusive fluxes must be zero:

\[ Q \rho w_k \mathbf{V}_k = 0 \quad (7-4) \]

An alternative is to use the fact that the sum of the mass fractions must be equal to one:

\[ w_Q = 1 - \sum_{k=1}^{Q-1} w_k \quad (7-5) \]

In the Heavy Species interface, Equation 7-5 is used to fulfill the mass constraint so only \( Q - 1 \) species are solved for.

**Source Coefficients**

The rate expression, \( R_k \) is determined by the stoichiometry of the system through the formula

\[ c_k = \frac{w_k \rho}{M_k} \]
\[ R_k = M_k \sum_{j=1}^{N} v_{kj} r_j \]  

(7-6)

where \( v_{kj} \) is the stoichiometric matrix and \( r_j \) is the reaction rate corresponding to reaction \( j \). The reaction rates depend on the order of the reaction and the molar concentration of each species. In compact form, the equation for the \( j \)th reaction rate is

\[
   r_j = \frac{k_{f,j}}{M_k} \prod_{k=1}^{Q} c_k^{v_{kj}} - \frac{k_{r,j}}{M_k} \prod_{k=1}^{Q} c_k^{v_{kj}}
\]

where:

- \( c_k \) is the molar concentration of species \( k \) (SI unit: mol/m\(^3\))
- \( k_{f,j} \) is the rate coefficient for the \( j \)th forward reaction (SI unit: 1/s, mol/(m\(^3\)s) or mol\(^2\)/(m\(^6\)s))
- \( v_{kj} \) is the stoichiometric matrix corresponding to forward reactions, and
- \( v_{kj} \) is the stoichiometric matrix corresponding to reverse reactions.

The molar concentration of the \( k \)th species is computed via:

\[
   c_k = \frac{w_k \rho}{M_k}.
\]

The rate coefficients \( k_j \) depend exponentially on the gas temperature through Arrhenius law

\[
   k_j = A_j T^\beta \exp \left( \frac{E_j}{RT} \right)
\]

where \( A_j \) is the frequency factor for reaction \( j \), \( \beta \) is the temperature exponent and \( E_j \) is the activation energy for reaction \( j \).

**Thermodynamic Properties**

The species’ heat capacity, \( C_p \), the molar enthalpy, \( h \), and the molar entropy, \( s \), are computed using the polynomial format of Gordon and McBride (Ref. 1). This manual also refers to these expressions as NASA polynomials:

\[
   C_{p,i} = R_i \left( a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \right)
\]

(7-7)
Here, $C_{p,i}$ denotes the species’ heat capacity (SI unit: J/(mol·K)), $T$ the temperature (SI unit: K), and $R_g$ the ideal gas constant, 8.314 J/(mol·K). Further, $h_i$ is the species’ molar enthalpy (SI unit: J/mol), and $s_i$ represents its molar entropy (SI unit: J/(mol·K)), at standard state.

The thermodynamic properties for a given reaction are computed from the enthalpy and entropy of the participating species. The enthalpy of reaction (SI unit: J/mol) is calculated using:

$$H_j = \sum_i v_{ij} h_i$$  \hspace{1cm} (7-10)$$

Similarly, the entropy of reaction (SI unit: J/(mol·K)) comes from the relationship

$$S_j = \sum_i v_{ij} s_i$$  \hspace{1cm} (7-11)$$

In these equations, $h_i$ and $s_i$ are the species’ molar enthalpy (SI unit: J/mol) and entropy (SI unit: J/(mol·K)), respectively. The heat source of reaction (SI unit: J/(m³·s)) is given as:

$$Q_j = -H_j r_j$$

The sum of $Q_j$ over all reactions is the total heat source due to chemical reaction:

$$Q = \sum_j Q_j$$

**Species Transport Properties**

The diffusion coefficients are computed from the following expression based on kinetic gas theory:

$$D_{kj} = 2.66 \cdot 10^{-2} \cdot \sqrt{T^3(M_k + M_j)/(2 \cdot 10^3 M_k M_j)} \cdot \frac{1}{\rho \sigma_k \sigma_j \Omega_D}$$  \hspace{1cm} (7-12)$$
Here:

- \( D_{kj} \) is the binary diffusion coefficient (SI unit: \( \text{m}^2/\text{s} \))
- \( M \) equals the molecular weight (SI unit: \( \text{kg/mol} \))
- \( T \) represents the temperature (SI unit: \( \text{K} \))
- \( p \) is the pressure (SI unit: \( \text{Pa} \)), and
- \( \sigma \) equals the characteristic length (SI unit: \( \text{Å} \)) of the Lennard-Jones/Stockmayer potential.

In addition, \( \Omega_D \) is the collision integral, given by the following equation (Ref. 2 and Ref. 3):

\[
\Omega_D = A(T^*)^{-B} + C[\exp(-DT^*)] + E[\exp(-FT^*)]
+ G[\exp(-HT^*)] + \frac{0.19\delta_{kji}^2}{T^*}
\tag{7-13}
\]

where

\[
T^* = \frac{k_B T}{\varepsilon_{kj}}
\]

\[
\varepsilon_{kj} = (\varepsilon_k \varepsilon_j)^{1/2}
\]

\[
\delta_{kj} = (\delta_k \delta_j)^{1/2}
\]

\[
\sigma_{kj} = (\sigma_k \sigma_j)^{1/2}
\]

\[
\delta = \frac{1}{2} \frac{\mu^2}{\varepsilon \sigma^3}
\tag{7-14}
\]

In Equation 7-14, \( \mu \) is the species dipole moment (SI unit: Debye). For gases at moderate pressure, the binary diffusivity can be used for the multicomponent Maxwell-Stefan diffusivities.

The predefined expression for the dynamic viscosity is given by the kinetic gas theory (Ref. 2 and Ref. 3) as

\[
\mu_i = 2.669 \cdot 10^{-6} \frac{T(M_i \cdot 10^3)}{\sigma_i^2 \Omega_v}
\tag{7-15}
\]
Here $\mu$ represents the dynamic viscosity (SI unit: Ns/m$^2$), and $\Omega_v$ is the collision integral, given by

$$\Omega_v = A(T^*)^{-B} + C[\exp(-DT^*)] + E[\exp(-FT^*)] + \frac{0.20\delta^2}{T^*}$$

with

$$T^* = \frac{T}{\epsilon}$$
$$\delta = \frac{1}{2}\frac{\mu^2}{\epsilon\sigma^3}$$

In Equation 7-16, $\mu$ is the species dipole moment (SI unit: Debye). The predefined expression for thermal conductivity comes from the Stiel-Thodos equation (Ref. 4)

$$k = \frac{n}{M}(1.15C_p + 0.88\gamma_g)$$

where the thermal conductivity $k$ is in (SI unit: W/(m·K)). Here $C_p$ denotes the heat capacity (SI unit: J/(mol·K)).

**Mixture Transport Properties**

The transport properties of the mixture are computed using the following for specific heat capacity (SI unit: J/(kg·K))

$$c_{p,mix} = \frac{\sum x_iC_{p,i}}{\sum x_iM_i}$$

The thermal conductivity (SI unit: W/(m·K)) is computed using:

$$k_{mix} = \frac{1}{2}\left[\sum x_ik_i + \left(\sum \frac{x_i}{k_i}\right)^{-1}\right]$$

In these equations:

- $T$ is the temperature (SI unit: K)
- $x$ is the mole fraction
• $M$ is the molecular weight (SI unit: kg/mol)
• $c_p$ is the heat capacity per unit mass (SI unit: J/(kg·K))
• $C_p$ represents the heat capacity per mole (SI unit: J/(mol·K)), and
• $k$ is the thermal conductivity (SI unit: W/(m·K)).

The dynamic viscosity (SI unit: Ns/m$^2$) is computed using:

$$\mu_{\text{fluid}} = \sum_{i=1}^{x} x_i \mu_i \sum_{j=1}^{\phi_{ij}}$$

where

$$\phi_{ij} = \left[ 1 + \left( \frac{\eta_i}{\eta_j} \right)^{0.5} \right] \left( \frac{M_i}{M_j} \right)^{0.25}$$

In these equations $\mu$ denotes the dynamic viscosity (SI unit: Ns/m$^2$).

**Scaling**

Because there can be a large variation in mass fraction of the components of a plasma, a logarithmic scaling of the equations is sometimes necessary. So, starting with the equation for a generalized mass transport template

$$\rho \frac{\partial}{\partial t} (w_k) + \rho (\mathbf{u} \cdot \nabla) w_k = \nabla \cdot (\rho w_k \mathbf{V}_k) + R_k$$  \hspace{1cm} (7-18)$$

and letting $W_k = \ln w_k$, Equation 7-18 becomes

$$\rho w_k \frac{\partial}{\partial t} (W_k) + \rho w_k (\mathbf{u} \cdot \nabla) W_k = \nabla \cdot (\rho w_k \mathbf{V}_k) + R_k$$

The first term on the right-hand side depends on which formulation is used. For the Mixture averaged diffusion model:

$$\mathbf{V}_k = D_{k,m} \nabla w_k + D_{k,m} \nabla \ln M + D^T \nabla \ln T - Z_k \mu_{k,m} \mathbf{E}$$

and for the Fick’s law diffusion model:
\[ V_k = D_k,f \nabla W_k + D_k,f \nabla \ln M + D^T \nabla \ln T - Z_k \mu_k, f E. \]

You can switch between the standard and logarithmic formulations of the mass balance equation. In this module the default implementation is logarithmic.

**Stabilization**

When the source stabilization is on, an additional term is added to the rate expression, Equation 7-6. The expression takes the form:

\[ R_{k,\text{tot}} = R_k + \exp(-1 \ln(n_k)) \]

where \( t \) is the user-defined tuning parameter. When the species number density is very low, this acts as a source term which prevents the mass fraction from approaching zero. As the number density increases this term becomes exponentially smaller, eventually becoming negligible for high number densities.

**Surface Reactions**

The equations solved for the transport for each species need to be supplemented by appropriate boundary conditions. This is often accomplished by way of a set of suitable surface reactions, which describe how species are created or consumed on surfaces. Assume a surface mechanism with \( I \) surface reactions and \( K \) chemical species

\[
\sum_{k=1}^{K} v_{k,i} c_k = \sum_{k=1}^{K} v_{k,i}^r c_k^r
\]

where \( v_{k,i} \) are the stoichiometric coefficients and \( c_k \) is the concentration of the \( k \)th species. The surface rate expression (SI unit: mol/(m\(^2\cdot\)s)) for species \( k \) is defined as

\[
R_{\text{surf},k} = \sum_{i=1}^{I} v_{k,i} q_i
\]

where \( v_{k,i} = v_{k,i}^r - v_{k,i}^f \). The rate of progress of the \( i \)th reaction is governed by the law of mass action:

\[
q_i = k_{f,i} \prod_{k=1}^{K} c_k^{f_{r,k,i}} - k_{r,i} \prod_{k=1}^{K} c_k^{r_{r,k,i}}
\]
where the following definitions apply for \( c_k \).

**Gas Phase Species**

The molar concentration is given by:

\[
e_k = \frac{w_k \rho}{M_k}
\]

where \( w_k \) is the mass fraction of species \( k \), \( \rho \) is the gas density, and \( M_k \) is the molecular weight of species \( k \). When the Motz-Wise correction option is set to On, the forward rate constant is related to the sticking coefficients via:

\[
k_{f, i} = \left( \frac{\gamma_i}{1 - \gamma_i / 2} \right) \frac{1}{(\Gamma_{tot})^m} \left( \frac{1}{\gamma_i} \right) \frac{SRT}{\pi M_n}
\]

When the Motz-Wise correction option is set to Off, the forward rate constant is given via:

\[
k_{f, i} = \frac{\gamma_i}{(\Gamma_{tot})^m} \left( \frac{1}{\gamma_i} \right) \frac{SRT}{\pi M_n}
\]

where \( \Gamma_{tot} \) is the total surface site concentration (SI unit: mol/m\(^2\)). The sticking coefficient can be a constant or even temperature dependent through an Arrhenius expression:

\[
\gamma_i = a_i T^b \exp \left( -\frac{e_i}{RT} \right)
\]

where \( a, b, \) and \( e \) are constants. Since \( \gamma \) is a probability it must be between 0 and 1 to be physically meaningful.

**Flux Matching**

Flux matching must be performed for each species in order for the total molar mass in the system to be conserved. If a model also contains a physics interface to compute the fluid velocity and pressure (the Laminar Flow interface for example) and the gas temperature (the Heat Transfer in Fluids interface for example) then those interfaces require appropriate flux matching boundary conditions. The Heavy Species interface
automatically computes flux matching variables for the total mass flux and heat source of reaction on surfaces.

**FLUX MATCHING FOR EACH SPECIES**

The inward mass flux for species $k$ on a reacting surface is given by:

$$-\mathbf{n} \cdot \mathbf{j}_k = M_k R_{\text{surf}, k}$$  \hspace{1cm} (7-21)

This is the natural boundary condition for Equation 7-3 and results in either an inwards or outward mass flux for species $k$, depending on the surface chemical mechanism stoichiometry. If the species is an ion, then there is an additional flux contribution due to migration. In this case, Equation 7-21 becomes:

$$-\mathbf{n} \cdot \mathbf{j}_k = M_k R_{\text{surf}, k} + M_k c_k u_{m,k} z_k (\mathbf{n} \cdot \mathbf{E}) \left[ (z_k \mathbf{n} \cdot \mathbf{E}) > 0 \right]$$

This additional flux contribution ensures that when the normal electric field is directed to the wall, there is an outflux of ions due to migration.

**FLUX MATCHING FOR THE TOTAL MASS FLUX**

If a model contains the Laminar Flow interface, an expression for the mass averaged velocity is needed on reacting surfaces. The Heavy Species interface creates an appropriate variable for the inward mass flux, which can be accepted as a feature input for the Mass Flow option in the Inlet boundary condition of the Laminar Flow interface.

The inward mass flux, $M_f$ is defined as:

$$M_f = \sum_{k=1}^{K_f} M_k R_{\text{surf}, k}$$

where $R_{\text{surf}, k}$ is the surface rate expression for each species which comes from summing the surface reaction rates multiplied by their stoichiometric coefficients over all surface reactions.
FLUX MATCHING FOR THE TOTAL HEAT FLUX

If a model contains the Heat Transfer in Fluids interface, an expression for the total heat source of reactions is needed. The Heavy Species interface creates an appropriate variable for the total heat source of reactions, which can be accepted as a feature input in the Reaction Heat Flux boundary condition of the Heat Transfer in Fluids interface.

The total heat source due to reactions is defined as:

$$Q_b = \sum_{i=1}^{I} q_i h_i$$

where \( h_i \) is the molar enthalpy change due to reaction \( i \). Depending on the surface chemical mechanism stoichiometry, this can either cause heating (exothermic) or cooling (endothermic).

About Surface Species

For each of the \( k \) Surface Species the following equations are solved:

$$\frac{d\Gamma_k}{dt} = \sum_{i=1}^{N} q_i \Delta\sigma_i$$

where \( \Gamma_k \) is the surface site concentration (SI unit: mol/m\(^2\)), \( q_i \) is the reaction rate for reaction \( i \) (SI unit: mol/m\(^2\)), and \( \Delta\sigma_i \) is the change in site occupancy number for reaction \( i \) (dimensionless).

$$\frac{dZ_k}{dt} = \frac{R_{\text{surf},k}}{\Gamma_{\text{tot}}}$$

where \( Z_k \) is the site fraction (dimensionless), and \( R_{\text{surf},k} \) is the surface rate expression (SI unit: mol/m\(^2\)). The quantity \( Z_k \) is the surface equivalent of the mole fraction on the volumetric level. That is, the sum of the site fractions must always equal one:

$$\sum Z_k = 1$$
For each of the bulk surface species, the following equation is solved for the deposition height:

\[
\frac{dh_k}{dt} = \frac{R_{\text{surf}, k} M_k}{\rho_k}
\]

where \( h_k \) is the total growth height (SI unit: m), \( M_k \) is the molecular weight (SI unit: kg/mol), and \( \rho \) is the density of the bulk species (SI unit: kg/m\(^3\)).

**Limitations of the Heavy Species Transport Equations**

Before continuing, some comments on the validity of the equations are necessary. Despite their relatively complicated form, the equations for transport of the heavy species are formulated under the following assumptions:

- The diffusion velocity must be much less than the thermal velocity; that is, \( V_k \ll v_k \).
  In the case of very low pressure CCP reactors, the ion drift velocity can approach or exceed the ion thermal velocity. In this case, the heavy species transport equations fail to fit the physics of the discharge.
- A single temperature is assumed for heavy species. In the case of reactors with high reduced electric fields, the ions can have a different temperature than the surrounding gas.

**References for the Heavy Species Transport Interface**


The Plasma Reactor Interfaces

This chapter describes three of the Plasma Module multiphysics interfaces found under the Plasma branch when adding a physics interface.

In this chapter:

- The Capacitively Coupled Plasma Interface
- The DC Discharge Interface
- The Inductively Coupled Plasma Interface
- The Microwave Plasma Interface
- Plasma Reactors Theory
- Theory for the Capacitively Coupled Plasma Interface
- Theory for the DC Discharge Interface
- Theory for the Inductively Coupled and Microwave Plasma Interfaces
The Capacitively Coupled Plasma Interface

The Capacitively Coupled Plasma (ccp) interface ( ), found under the Plasma branch ( ) when adding a physics interface, couples the Drift Diffusion, Heavy Species Transport, and Electrostatics interfaces into an integrated multiphysics interface to model capacitively coupled plasma (CCP). It is used to study discharges that are sustained by a time-varying electrostatic field.

When this interface is added, these default nodes are also added to the Model Builder—Plasma Model, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Capacitively Coupled Plasma to select physics from the context menu.

INTERFACE IDENTIFIER

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

The default identifier (for the first interface in the model) is ccp.

DOMAIN SELECTION

The default setting is to include All domains in the model to define the dependent variables and the equations for the plasma discharge. To choose specific domains, select Manual from the Selection list.

Except where described in this section, this interface shares it physics nodes with The Drift Diffusion Interface, The Heavy Species Transport Interface, and The Electrostatics Interface.
TRANSPORT SETTINGS
Select a **Diffusion model**—**Mixture-averaged** (the default) or **Fick’s law**. When using the **Mixture-averaged** model, the mixture averaged diffusion coefficients are automatically computed based on the data specified for each species.

Select the check boxes for which transport mechanisms to **Include**—**Convection**, **Migration in electric field**, **Calculate thermodynamic properties**, **Full expression for diffusivity**, or **Compute tensor ion transport properties**. The selection changes the number of **Model Inputs** requiring values on the **Plasma Model** page. Note the following:

- The **Migration** term is part of the relative mass flux vector.
- **Convection** of heavy species present in a plasma can often be neglected due to the low operating pressure.
- If **Calculate thermodynamic properties** is selected, select that the thermodynamic properties of each reaction and species are computed automatically based on the thermodynamic properties of each species.
- If **Full expression for diffusivity** is selected, it computes a more accurate expression for the Maxwell-Stefan diffusivities. Often the additional correction terms are negligible in which case the expressions are much simpler and the time taken to assemble the Jacobian matrix is reduced.
- If the **Compute tensor ion transport properties** option is selected, the tensor form of the ion transport properties when a static magnetic field is present is computed. This option only needs to be activated when a strong DC magnetic field exists and the operating pressure is very low (on the order of millitorr). When this option is activated an expression must be provided for the magnetic flux density, which typically another physics interface computes. This is set in the **Plasma Model** node.

PLASMA PROPERTIES
Select the **Compute tensor electron transport properties**, **Use reduced electron transport properties** and **Fix mean electron energy** check boxes as required.

Select **Compute tensor electron transport properties** to compute the tensor form of the electron mobility, electron diffusivity, energy mobility and energy diffusivity. This should only be used in cases where a strong DC magnetic field exists. Two quantities must be supplied, both of which are in the **Plasma Model** node. The DC mobility which is the value of the electron mobility in the absence of a DC magnetic field and the magnetic flux density which would typically be computed by another physics interface.
Select **Use reduced electron transport properties** to specify the electron mobility, diffusivity, energy mobility and energy diffusivity in reduced form. The neutral number density is then specified in the Drift Diffusion Model node. The electron transport properties are computed from the reduced transport properties using:

\[ \mu_e = \frac{\mu_{\text{red}}}{N_n} \]

where \( N_n \) is the user-defined neutral number density.

The **Include thermal diffusion** check box adds an additional term to the definition of the electron current due to gradients in the electron diffusivity. If the diffusivity is a constant then including this does not affect the solution. It is only necessary to include this term if the electron diffusivity is a function of the electron temperature, and there are significant gradients in the electron temperature.

Select **Fix mean electron energy** to fix the mean electron energy to its initial value. This can be useful in some situations because the strong coupling between the mean electron energy and the electromagnetic fields is removed. This allows for non-self consistent models to be created quickly, since problems where the mean electron energy is fixed are easier to solve numerically.

The Inductively Coupled Plasma Interface and The Microwave Plasma Interface have an additional option to **Compute tensor plasma conductivity**. If there is a strong DC magnetic field present then the plasma conductivity becomes a full tensor and a highly nonlinear function of the magnetic flux density. If this option is selected, COMSOL Multiphysics automatically computes the tensor form of the plasma conductivity based on the conductivity and magnetic flux density specified in the Plasma Model node.

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For details on the implementation, see **Plasma Conductivity in the Presence of a Static Magnetic Field**.

For more information on the electron energy distribution function (EEDF), see the **Theory for the Boltzmann Equation, Two-Term Approximation Interface**.

---

**ELECTRON ENERGY DISTRIBUTION FUNCTION**

If cross section data is used to define source coefficients in the model then an electron energy distribution function (EEDF) needs to be selected. Select one of these options.

- **Maxwellian**. This option assumes a Maxwellian EEDF which takes the form:
\[ f(\varepsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\varepsilon \beta_2 / \varphi\right) \]

where

\[ \beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1} \]

where \( \varphi \) is the mean electron energy (SI unit: eV), \( \varepsilon \) is the electron energy (SI unit: eV) and \( \Gamma \) is the incomplete gamma function.

- **Druyvesteyn.** This option assumes a Druyvesteyn EEDF which takes the form:

\[ f(\varepsilon) = 2\varphi^{-3/2} \beta_1 \exp\left(-\varepsilon \beta_2 / \varphi\right)^2 \]

where

\[ \beta_1 = \Gamma(5/4)^{3/2} \Gamma(3/4)^{-5/4}, \beta_2 = \Gamma(5/4) \Gamma(3/4)^{-1} \]

- **Generalized.** Use this option for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. If this option is selected, specify a power law. This number must be between 1 and 2. Mathematically, the EEDF takes the form:

\[ f(\varepsilon) = g \varphi^{-3/2} \beta_1 \exp\left(-\varepsilon \beta_2 g / \varphi\right)^g \]

where

\[ \beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g) \Gamma(3/2g)^{-1}, 1 \leq g \leq 2 \]

- **Function.** If a two dimensional interpolation function has been added to the model, it can be used for the EEDF. In this case, the x-data should be the electron energy (eV) and the y-data should be the mean electron energy (eV).

---

The two dimensional interpolation function can be computed using a parametric sweep in The Boltzmann Equation, Two-Term Approximation Interface. This allows for modeling of discharges where the EEDF is far from Maxwellian. See Interpolation in the COMSOL Multiphysics Reference Manual.

In all these cases the rate constants in the model are automatically computed based on the selected EEDF using the formula:
The rate coefficients when computed using cross section data are a highly nonlinear function of the mean electron energy. COMSOL Multiphysics automatically computes the integral in Equation 8-1 and makes the result available for evaluation of the rate coefficient. The variation of the rate coefficient for any particular model can be plotted using `<interface identifier>.kf_<reaction number>`. For example, for reaction number 3 in a DC Discharges interface, with identifier dc, the rate coefficient is plotted using `dc.kf_3`.

**CHEMKIN**

Import thermodynamic and transport properties for the reacting species into the model.

The thermodynamic and transport input files must follow the CHEMKIN® standard.

**STABILIZATION**

If the Equation formulation is set to Log then the solver can run into difficulties as the species mass fractions approach zero. The Reaction source stabilization check box (selected by default) adds an additional source term to the rate expression for each species. In the $t$ field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

The solver can also run into difficulties as the electron density or electron energy density approach zero. The Source stabilization check box (selected by default) adds an additional source term to the equation for the electron density and electron energy density. In the $\zeta$ field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

**ADVANCED SETTINGS**

Select a Formulation—Finite element (the default) or Finite volume. The Finite element option uses the Galerkin method to discretize the equations whereas the Finite volume
option creates degrees of freedom for the dependent variables which are piecewise constant within each mesh element. For the charged species, Scharfetter-Gummel upwinding is used. For charge neutral species and the electrostatic field, a centered difference scheme is used. In cases where the ion and electron flux are strongly driven by the electric field, the finite volume option can be more stable. Examples where this is true include dielectric barrier and corona discharges.

When the formulation is set to finite element, select an equation formulation—log (the default) to solve the equations in logarithmic form or linear to solve equations in the original form. Log solves for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve.

**Dependent Variables**
The dependent variables (field variables) are the electron potential, log of electron density, and log of electron energy density. The name can be changed but the names of fields and dependent variables must be unique within a model.

**Discretization**
To display this section, click the Show button ( ) and select discretization. Select linear (the default), quadratic, cubic, or quartic for the log of electron density and log of electron energy density. Specify the value type when using splitting of complex variables—real or complex (the default).
CHAPTER 8: THE PLASMA REACTOR INTERFACES

Domain, Boundary, Edge, Point, and Pair Physics for the Capacitively Coupled Plasma Interface

The Capacitively Coupled Plasma Interface has these domain, boundary, edge, point, and pair nodes, listed in alphabetical order, 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. However, to add subnodes, right-click the parent node.

These physics are described in this section:

- Plasma Model
- Initial Values
- Continuity on Interior Boundary

These physics are described for the Drift Diffusion or Heavy Species Transport interface (listed in alphabetical order):

- Cross Section Import
- Electron Density and Energy
- Electron Impact Reaction
- Electron Outlet
- Electron Production Rate
- Flux
- General Power Deposition
- Insulation
- Reaction
- Species
- Surface Reaction
- Surface Species
- Velocity
- Wall
These physics are described for the Electrostatics interface (listed in alphabetical order):

- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- External Surface Charge Accumulation
- Floating Potential
- Ground
- Line Charge
- Periodic Condition
- Point Charge
- Surface Charge Accumulation
- Surface Charge Density
- Terminal
- Thin Low Permittivity Gap
- Zero Charge

In the COMSOL Multiphysics Reference Manual:
- Continuity on Interior Boundaries
- Identity and Contact Pairs

**Plasma Model**

Use the Plasma Model node to set the electron transport properties, material properties, and model inputs.

**Domain Selection**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

**Model Inputs**

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs display here. Initially, this section is empty. The input depends on which Transport Settings are selected on the Capacitively Coupled Plasma or DC Discharges interfaces.
• Enter a Temperature $T$ (SI unit: K) for the gas mixture used to compute the gas density and species transport properties.

• Enter an Absolute pressure $p$ (SI unit: Pa) to compute the gas density and the Maxwell-Stefan diffusivities.

• If the Convection check box is selected, enter coordinates for the Velocity field $\mathbf{u}$ (SI unit: m/s).

• If the Compute tensor electron transport properties or the Compute tensor ion transport properties property is activated enter an expression for the Magnetic flux density $B$ (SI unit: T). This usually comes from a magnetostatic model, and is used to compute anisotropic transport properties for electrons and ions.

**Density**

Select an option from the Mixture density list—Ideal gas or User defined. If User defined is selected, enter a value for $\rho$ (SI unit: kg/m$^3$).

If Ideal gas is selected, it computes the expression for the gas density automatically using the ideal gas law, based on the composition of the mixture. The density is a function of the mean molecular weight:

$$\rho = \frac{p_A M}{R T}$$

where $p_A$ is the absolute pressure, $T$ is the temperature, $R$ is the universal gas constant and $M$ is the mean molecular weight given by:

$$\frac{1}{M} = \sum_{k=1}^{Q} \frac{w_k}{M_k}$$

**Electron Density and Energy**

Select an option from the Electron transport properties list—Specify mobility only (the default), Specify all, or Use lookup tables. The options available depend on whether the Use reduced electron transport properties interface property is checked. If the interface property Compute tensor electron transport properties is checked then only one field...
appears for the DC or reduced DC electron mobility, $\mu_{dc}$. The other transport properties are computed using Einstein’s relation.

Tensor Transport Properties

- If **Specify mobility only** is selected, enter a value or expression for the **Electron mobility** $\mu_e$ (SI unit: m$^2$/V·s). Select **Isotropic, Diagonal, Symmetric** or **Anisotropic** based on the model. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

$$D_e = \mu_e T_e, \quad \mu_e = \left(\frac{5}{3}\right) \mu_e, \quad D_e = \mu_e T_e$$

(8-2)

If the **Use reduced electron transport properties** interface property is checked then enter the **Reduced electron mobility** $\mu_e N_n$ (SI unit: sA/(m$^3$·kg)). The actual electron mobility is then computed by dividing the reduced electron mobility by the neutral number density.

- If **Specify all** is selected, enter values or expressions for all of the properties, which can be either scalars or tensors. The appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface. For all of the properties, select **Isotropic, Diagonal, Symmetric** or **Anisotropic** from the list based on the model, then enter values or expressions for all of these properties:

  - **Electron mobility** $\mu_e$ (SI unit: m$^2$/V·s)
  - **Electron diffusivity** $D_e$ (SI unit: m$^2$/s)
  - **Electron energy diffusivity** $D_{en}$ (SI unit: m$^2$/s)
  - **Electron energy mobility** $\mu_{en}$ (SI unit: m$^2$/V·s)

If the **Use reduced electron transport properties** interface property is selected then enter:

  - **Reduced electron mobility** $\mu_e N_n$ (SI unit: sA/(m$^3$·kg))
  - **Reduced electron diffusivity** $D_e N_n$ (SI unit: 1/(m·s))
  - **Reduced electron energy diffusivity** $D_{en} N_n$ (SI unit: 1/(m·s))
  - **Reduced electron energy diffusivity** $\mu_{en} N_n$ (SI unit: sA/(m$^3$·kg))
If **Use lookup tables** is selected, enter or load a lookup table with the transport properties as listed above versus mean electron energy (eV).

If the **Use reduced electron transport properties** interface property is selected, the appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface and written out to a text file. The text file can then be loaded in for each electron transport property.

### Initial Values

Use the **Initial Values** node to set the initial values of the electron density, mean electron energy, and electric potential.

Initial conditions for the heavy species are specified on the individual species features.

### Domain Selection

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select **Manual** from the **Selection** list to choose specific domains or select **All domains** as required.

### Initial Values

Enter values or expressions for each of the following:

- **Initial electron density** \( n_{e,0} \) (SI unit: \( 1/m^3 \)). This value represents some initial seed electrons in the plasma. If this number is too low then the plasma might not sustain itself. If this number is too high then numerical instabilities can arise at early time steps.

- **Initial mean electron energy** \( e_0 \) (SI unit: \( V \)). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess is set to the expected value the easier it is to find a solution.

- **Electric potential** \( V \) (SI unit: \( V \)). In nearly all cases the value should be zero. This initial value must also be consistent with any boundary conditions on the electric potential in the model.
Continuity on Interior Boundary

When the finite volume formulation is chosen, it might be necessary to enforce continuity in the electrical displacement on interior boundaries. The Continuity on Interior Boundary feature ensures that this occurs. It is only possible to add this feature on interior boundaries.
**The DC Discharge Interface**

The **DC Discharge** (dc) interface, found under the **Plasma** branch when adding a physics interface, couples the Drift Diffusion, Heavy Species Transport, and Electrostatics interfaces. It is used to study discharges that are sustained by a static electric field. Townsend coefficients can be used instead of rate coefficients for electron source terms.

When this interface is added, these default nodes are also added to the **Model Builder**—**Plasma Model**, **Zero Charge**, **Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click **DC Discharge** to select physics from the context menu.

**INTERFACE IDENTIFIER**

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

The default identifier (for the first interface in the model) is `dc`.

Except where described in this section, this interface shares it physics nodes with **The Electrostatics Interface**, **The Drift Diffusion Interface**, and **The Heavy Species Transport Interface**.
See The Capacitively Coupled Plasma Interface for the rest of the settings on this interface and for Initial Values and Plasma Model. Also see:

- Show More Physics Options
- Domain, Boundary, Edge, Point, and Pair Physics for the Capacitively Coupled Plasma Interface
- Plasma Reactors Theory
- Theory for the DC Discharge Interface
- Building a COMSOL Model in the COMSOL Multiphysics Reference Manual

DC Glow Discharge: model library path
Plasma_Module/Direct_Current_Discharges/positive_column_2d
The Inductively Coupled Plasma Interface

This interface is available for 2D and 2D axisymmetric models.

With an AC/DC Module license, this interface is also available in 3D. This also enables additional features that are available with the AC/DC Module, and described in the AC/DC Module User’s Guide.

The Inductively Coupled Plasma (icp) interface ( ), found under the Plasma branch ( ) when adding a physics interface, couples the Drift Diffusion, Heavy Species Transport, Electrostatics, and Magnetic Fields interfaces. It is used to study discharges that are sustained by induction currents. The induction currents are solved for in the frequency domain. The electron heating due to the induction currents is automatically handled by the software.

When this interface is added, these default nodes are also added to the Model Builder—Plasma Model, Magnetic Insulation, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Inductively Coupled Plasma to select physics from the context menu.

INTERFACE IDENTIFIER

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

The default identifier (for the first interface in the model) is icp.
SETTINGS

This section is available for 2D and 2D axisymmetric models.

Use the Components list to define the components of the magnetic vector potential to be solved for.

ADVANCED SETTINGS

Select an Equation formulation—Log (the default) to solve the equations in logarithmic form or Linear to solve equations in the original form. Log solves for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Magnetic vector potential, Magnetic vector potential components, Electric potential, Log of electron density, and Log of electron energy density. The name can be changed but the names of fields and dependent variables must be unique within a model.

DISCRETIZATION

To display this section, click the Show button ( ) and select Discretization. Select Linear (the default), Quadratic, or Cubic for the Magnetic vector potential, Electric...
potential, Log of electron density and Log of electron energy density. Specify the Value type when using splitting of complex variables—Real or Complex (the default).

- Domain, Boundary, Point, and Pair Physics for the Inductively Coupled Plasma Interface
- The Capacitively Coupled Plasma Interface
- Plasma Reactors Theory
- Theory for the Inductively Coupled and Microwave Plasma Interfaces

Domain, Boundary, Point, and Pair Physics for the Inductively Coupled Plasma Interface

The Inductively Coupled Plasma Interface has these 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 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. However, to add subnodes, right-click the parent node.
These nodes are described in this section:

- Collisionless Heating
- Gauge Fixing for A-field
- Initial Values
- Plasma Model

These nodes are described for the Drift Diffusion or Heavy Species Transport interface (listed in alphabetical order):

- Cross Section Import
- Electron Density and Energy
- Electron Impact Reaction
- Electron Outlet
- Electron Production Rate
- Flux
- General Power Deposition
- Insulation
- Reaction
- Species
- Surface Reaction
- Surface Species
- Velocity
- Wall
These nodes are described for the Electrostatics interface (listed in alphabetical order):

- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- External Surface Charge Accumulation
- Floating Potential
- Ground
- Line Charge
- Periodic Condition
- Space Charge Density
- Surface Charge Accumulation
- Surface Charge Density
- Terminal
- Thin Low Permittivity Gap
- Zero Charge

These nodes are described for the Magnetic Fields interface in the COMSOL Multiphysics Reference Manual (listed in alphabetical order):

- Ampère’s Law
- External Current Density
- Line Current (Out-of-Plane)
- Magnetic Field
- Magnetic Insulation
- Magnetic Potential
- Perfect Magnetic Conductor
- Surface Current
- Velocity (Lorentz Term)

For 3D models, that is, if you also have the AC/DC Module, see Domain, Boundary, Point, and Pair Nodes for the Magnetic Fields Interface in the AC/DC Module User’s Guide for other available Magnetic Fields features.

If you are also using the AC/DC Module for 2D and 2D axisymmetric models, some of the available nodes are only available for these space dimensions. For example, Multi-Turn Coil Domain and Single-Turn-Coil Domain are described for the Magnetic Fields interface. See the AC/DC Module User’s Guide for more information.
In the COMSOL Multiphysics Reference Manual:

- Continuity on Interior Boundaries
- Identity and Contact Pairs
- Destination Selection
- Periodic Boundary Conditions

**Plasma Model**

Use the **Plasma Model** node to set the electron transport properties, material properties, and model inputs.

With the AC/DC Module (for a 3D Inductively Coupled Plasma interface) or the RF Module (for the Microwave Plasma interface), right-click the **Plasma Model** node to add a **Gauge Fixing A** or **Gauge Fixing D** node.

Most of the settings are the same for the Inductively Coupled Plasma and Microwave Plasma interfaces as for the Capacitively Coupled Plasma interface with two additional sections—**Magnetic Field** and **Conduction Current**.

**Domain Selection**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select **Manual** from the **Selection** list to choose specific domains or select **All domains** as required.

**Model Inputs**

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs display here. Initially, this section is empty. The input depends on which **Transport Settings** are selected on the Inductively Coupled Plasma or Microwave Plasma interfaces.

- Enter a **Temperature** $T$ (SI unit: K) for the gas mixture used to compute the gas density and species transport properties.
• Enter an **Absolute pressure** \( p \) (SI unit: Pa) to compute the gas density and the Maxwell-Stefan diffusivities.

• If the **Convection** check box is selected, enter coordinates for the **Velocity field** \( u \) (SI unit: m/s).

• If the **Compute tensor electron transport properties** or the **Compute tensor ion transport properties** property is activated enter an expression for the **Magnetic flux density** \( B \) (SI unit: T). This usually comes from a magnetostatic model, and is used to compute anisotropic transport properties for electrons and/or ions.

### Density
Select an option from the **Mixture density** list—**Ideal gas** or **User defined**. If **User defined** is selected, enter a value for \( \rho \) (SI unit: kg/m\(^3\)).

If **Ideal gas** is selected, it computes the expression for the gas density automatically using the ideal gas law, based on the composition of the mixture. The density is a function of the mean molecular weight:

\[
\rho = \frac{p_A M_n}{RT}
\]

where \( p_A \) is the absolute pressure, \( T \) is the temperature, \( R \) is the universal gas constant and \( M \) is the mean molecular weight given by:

\[
\frac{1}{M_n} = \sum_{k=1}^{Q} \frac{w_k}{M_k}
\]

### Electron Density and Energy
Select an option from the **Electron transport properties** list—**Specify mobility only** (the default), **Specify all**, or **Use lookup tables**. The options available depend on whether the **Use reduced electron transport properties** interface property is checked. If the interface property Compute tensor electron transport properties is checked then only one field appears for the DC or reduced DC electron mobility, \( \mu_{dc} \). The other transport properties are computed using Einstein’s relation.
• If Specify mobility only is selected, enter a value or expression for the Electron mobility $\mu_e$ (SI unit: $m^2/(V\cdot s)$). Select Isotropic, Diagonal, Symmetric or Anisotropic based on the model. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

$$D_e = \mu_e T_e, \quad \mu_e = \left(\frac{5}{3}\right)\mu_e, \quad D_e = \mu_e T_e$$ (8-3)

If the Use reduced electron transport properties interface property is checked then enter the Reduced electron mobility $\mu_eN_n$ (SI unit: $sA/(m^3\cdot kg)$). The actual electron mobility is then computed by dividing the reduced electron mobility by the neutral number density.

• If Specify all is selected, enter values or expressions for all of the properties, which can be either scalars or tensors. The appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface. For all of the properties, select Isotropic, Diagonal, Symmetric or Anisotropic from the list based on the model, then enter values or expressions for all of these properties:
  - Electron mobility $\mu_e$ (SI unit: $m^2/(V\cdot s)$)
  - Electron diffusivity $D_e$ (SI unit: $m^2/s$)
  - Electron energy diffusivity $D_en$ (SI unit: $m^2/s$)
  - Electron energy mobility $\mu_en$ (SI unit: $m^2/(V\cdot s)$)

If the Use reduced electron transport properties interface property is checked then enter:
  - Reduced electron mobility $\mu_eN_n$ (SI unit: $sA/(m^3\cdot kg)$)
  - Reduced electron diffusivity $D_eN_n$ (SI unit: $1/(m\cdot s)$)
  - Reduced electron energy diffusivity $D_enN_n$ (SI unit: $1/(m\cdot s)$)
  - Reduced electron energy diffusivity $\mu_enN_n$ (SI unit: $sA/(m^3\cdot kg)$)

If Use lookup tables is selected, enter or load a lookup table with the transport properties as listed above versus mean electron energy (eV).

If the Use reduced electron transport properties interface property is selected, the appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface and written out to a text file. The text file can then be loaded in for each electron transport property.
**Collisionless Heating**

The Collisionless Heating node includes the non-local heating effects via an effective viscosity approximation. Typically this is only important at very low pressures (less than 2 Pa) and frequencies above 10 MHz.

**Domain Selection**

This setting has no initial selection. Select the domains where the collisionless heating should be applied. Typically this should be the domains where the Plasma Model feature is applied.

**Initial Values**

Use the Initial Values node to set the initial values of the electron density, mean electron energy, electric potential, and magnetic vector potential. Set the initial values of the heavy species on each species feature.

**Domain Selection**

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.

**Initial Values**

Enter values or expressions for each of the following:

- **Initial electron density** $n_{e,0}$ (SI unit: $1/m^3$). This value represents some initial seed electrons in the plasma. If this number is too low then the plasma might not sustain itself. If this number is too high then numerical instabilities can arise at early time steps.

- **Initial mean electron energy** $e_0$ (SI unit: V). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess can be set to the expected value the easier it is to find a solution.

- **Electric potential** $V$ (SI unit: V). In nearly all cases the value should be zero. This initial value must also be consistent with any boundary conditions on the electric potential in the model.

- **Magnetic vector potential** $A$ (SI unit: $Wb/m$). The default value is zero and usually does not require changing.
Gauge Fixing for A-field

This node is normally only available with the addition of an AC/DC Module license. However, for a 2D model using The Inductively Coupled Plasma Interface, this node is available.

Right-click the Ampère’s Law node to add the Gauge Fixing for A-Field subnode. The feature provides gauge fixing by adding an additional potential variable, ψ, and its associated conservation equation to the system. This is often necessary to get a unique and numerically stable solution to the equation solving for the magnetic vector potential A.

Domain Selection

From the Selection list, choose the domains to define.

Gauge Fixing for A-field

Enter a Divergence condition variable scaling ψ0 (SI unit: A/m). The default value is 1 A/m, which means no scaling.

For more details on gauge fixing see Explicit Gauge Fixing/Divergence Constraint in the AC/DC Module User’s Guide.

The links to physics nodes described in other user’s guides or reference manuals do not work in the PDF, only from the on line help.
The Microwave Plasma Interface

**The Microwave Plasma (mwp) interface**, found under the Plasma branch when adding a physics interface, couples the Drift Diffusion, Heavy Species Transport, Electrostatics and Electromagnetic Waves interfaces. The interface is suitable for studying discharges that are sustained by electromagnetic waves (wave-heated discharge). Heating of the electrons due to their interaction with the electromagnetic waves is automatically handled by the software. The electromagnetic waves are solved for in the frequency domain.

When this interface is added, these default nodes are also added to the **Model Builder**—Plasma Model, Perfect Electric Conductor, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Microwave Plasma to select physics from the context menu.

Except where described in this section, this interface shares its physics nodes with The Drift Diffusion Interface, The Heavy Species Transport Interface, and The Electrostatics Interface as described in this guide and The Electromagnetic Waves, Frequency Domain Interface as described in the RF Module User’s Guide.

**INTERFACE IDENTIFIER**

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

The default identifier (for the first interface in the model) is mwp.
**SETTINGS**

Select the vector representing the components of the electric field to solve for:

- If **Three-component vector** is selected the in-plane and out-of-plane components of the electric field are computed. Vector elements are used for the in-plane components and Lagrange elements for the out-of-plane components. Use this vector to study the TEM mode. This is the default setting.

- If **Out-of-plane vector** is selected then only the out of plane component of the electric field is computed, the z-component in 2D and the φ-component in the axisymmetric case. This corresponds to the TE mode, and Lagrange elements are used for the out-of-plane electric field.

- If **In-plane vector** is selected then the in-plane components of the electric field are computed. This corresponds to the TM mode, and vector elements are used for the in-plane electric field.

**ADVANCED SETTINGS**

Select an **Equation formulation**—**Log** (the default) to solve the equations in logarithmic form or **Linear** to solve equations in the original form. **Log** solves for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve.

**DEPENDENT VARIABLES**

The dependent variables (field variables) are the **Electric field**, **Electric field components**, **Electric potential**, **Log of electron density**, and **Log of electron energy density**. The name can be changed but the names of fields and dependent variables must be unique within a model.

**DISCRETIZATION**

To display this section, click the **Show** button ( ) and select **Discretization**. Select **Linear** (the default), **Quadratic**, or **Cubic** for the **Electric field**, **Electric potential**, **Log of...**
**electron density** and Log of electron energy density. Specify the **Value type** when using splitting of complex variables—**Real** or **Complex** (the default).

- **Show More Physics Options**
- **The Inductively Coupled Plasma Interface**
- **Domain, Boundary, Point, and Pair Physics for the Inductively Coupled Plasma Interface**
- **Domain, Boundary, Edge, Point, and Pair Physics for the Microwave Plasma Interface**
- **Plasma Reactors Theory**
- **Theory for the Inductively Coupled and Microwave Plasma Interfaces**

- **In-Plane Microwave Plasma**: model library path
  `Plasma_Module/Wave_Heated_Discharges/inplane_microwave_plasma`

- **Dipolar Microwave Plasma Source**: model library path
  `Plasma_Module/Wave_Heated_Discharges/dipolar_ecr_source`

**Domain, Boundary, Edge, Point, and Pair Physics for the Microwave Plasma Interface**

The **Microwave Plasma 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. However, to add subnodes, right-click the parent node.

The physics interface shares most nodes and these are listed in **Domain, Boundary, Point, and Pair Physics for the Inductively Coupled Plasma Interface**, with the addition of the physics included with the RF Module license and those listed below.

These additional nodes are also available for this interface:

- **Initial Values**
Microwave Power Deposition (described for the Drift Diffusion interface)

Both the Electromagnetic Waves, Frequency Domain interface and its nodes are described in the RF Module User’s Guide as this interface requires the RF Module. For that reason, the following links do not work in the PDF but they do work in the on line help.

These nodes (and subnodes) are available for the Electromagnetic Waves, Frequency Domain interface and listed in alphabetical order.

- Divergence Constraint
- Edge Current
- Electric Field
- Electric Point Dipole
- Far-Field Domain
- Impedance Boundary Condition
- Line Current (Out-of-Plane)
- Lumped Port
- Magnetic Current
- Magnetic Field
- Magnetic Point Dipole
- Perfect Electric Conductor
- Perfect Magnetic Conductor
- Port
- Scattering Boundary Condition
- Surface Current
- Transition Boundary Condition
- Wave Equation, Electric

Initial Values

Use the Initial Values node to set the initial values of the electron density, mean electron energy, and electric potential.

Initial conditions for the heavy species are specified on the individual species features.

Domain Selection

For a default node, the setting inherits the selection from the parent node, and cannot be edited; that is, the selection is automatically selected and is the same as for the interface. When nodes are added from the context menu, you can select Manual from the Selection list to choose specific domains or select All domains as required.
INITIAL VALUES
Enter values or expressions for each of the following:

- **Initial electron density** $n_{e,0}$ (SI unit: $1/m^3$). This value represents some initial seed electrons in the plasma. If this number is too low then the plasma might not sustain itself. If this number is too high, numerical instabilities can arise at early time steps.

- **Initial mean electron energy** $e_0$ (SI unit: V). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess can be set to the expected value the easier it is to find a solution.

- **Electric potential** $V$ (SI unit: V). In nearly all cases the value should be zero. This initial value must also be consistent with any boundary conditions on the electric potential in the model.

- **Electric field** $E$ (SI unit: V/m). Enter a initial values for the components of the electric field. Any settings here must be consistent with any boundary conditions in the model. The default value of zero almost never needs changing.
The predefined plasma reactor interfaces couple the Drift Diffusion, Heavy Species and Electrostatic interfaces. A brief explanation of the underlying equations is given here.

For detailed information about electron transport see Theory for the Drift Diffusion Interface.

For detailed information about the transport of the non-electron species see Theory for the Heavy Species Transport Interface.

For detailed information about electrostatics see The Electrostatics Interface.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected.

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\mu_e \cdot E) - \nabla(D_e n_e)] = R_e
\]

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e(\mu_e \cdot E) - \nabla(D_e n_e)] + E \cdot \Gamma_e = R_e
\]

The electron source \( R_e \) and the energy loss due to inelastic collisions \( R_e \) are defined later. If a strong DC magnetic field is present then the electron mobility can be a tensor:

\[
\mu_e^{-1} = \begin{pmatrix}
\frac{1}{\mu_{de}} & -B_z & B_y \\
B_z & \frac{1}{\mu_{de}} & -B_x \\
-B_y & B_x & \frac{1}{\mu_{de}}
\end{pmatrix}
\]
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 \( \mu_{de} \) is the electron mobility in the absence of a magnetic field. The electron diffusivity, energy mobility and energy diffusivity are then calculated using:

\[
D_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{3} \right) \mu_{de}, \quad D_e = \mu_e T_e
\]

The source coefficients in the above equations are determined by the plasma chemistry and are written using either rate or Townsend coefficients. Suppose that there are \( M \) reactions which contribute to the growth or decay of electron density and \( P \) inelastic electron-neutral collisions. In general \( P \gg M \). In the case of rate coefficients, the electron source term is given by

\[
R_e = \sum_{j=1}^{M} x_j k_j N_n n_e
\]

where \( x_j \) is the mole fraction of the target species for reaction \( j \), \( k_j \) is the rate coefficient for reaction \( j \) (SI unit: \( m^3/s \)), and \( N_n \) is the total neutral number density (SI unit: \( 1/m^3 \)). When Townsend coefficients are used, the source term becomes

\[
R_e = \sum_{j=1}^{M} x_j \alpha_j N_n \Gamma_e
\]

where \( \alpha_j \) is the Townsend coefficient for reaction \( j \) (SI unit: \( m^2 \)) and \( \Gamma_e \) is the electron flux (SI unit: \( 1/(m^2 s) \)). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

The electron energy loss is obtained by summing the collisional energy loss over all reactions:

\[
R_e = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta \varepsilon_j
\]

where \( \Delta \varepsilon_j \) is the energy loss from reaction \( j \) (SI unit: \( V \)). In the case of Townsend coefficients, the energy loss is given by
The electron source and inelastic energy loss are automatically computed by the multiphysics interface. The rate coefficients can be computed from cross section data by the following integral:

$$ k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon) f(\varepsilon) d\varepsilon $$

where:

- $\gamma = (2q/m_e)^{1/2} (C/\text{kg}^{1/2})$
- $m_e$ is the electron mass (SI unit: kg)
- $\varepsilon$ is the energy (SI unit: V)
- $\sigma_k$ is the collision cross section (SI unit: m$^2$), and
- $f$ is the electron energy distribution function. Choose between Maxwellian, Druyvesteyn, or a Generalized EEDF.

For non-electron species, the following equation is solved for the mass fraction of each species.

$$ \rho \frac{\partial w_k}{\partial t} + \rho (\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k $$

The electrostatic field is computed using the following equation:

$$ -\nabla \cdot \varepsilon_0 \varepsilon_r \nabla \mathbf{V} = \rho $$

The space charge density, $\rho$ is automatically computed based on the plasma chemistry specified in the model using the formula:

$$ \rho = q \left( \sum_{k=1}^{N} Z_k n_k - n_e \right) $$

The Inductively Coupled Plasma interface also contains an equation for the high frequency component of the current. The Microwave Plasma interface solves an additional equation for the high frequency component of the electric field.
Theory for the Capacitively Coupled Plasma Interface

Capacitively coupled plasmas (CCP) represent a monumental challenge when it comes to numerical modeling for the following reasons:

- The method of power deposition into the plasma from the electric field is a highly nonlinear process meaning that the problem must be solved in the time domain. This requires the RF cycle to be accurately resolved over time. Because a capacitively coupled plasma can take thousands of RF cycles to reach a periodic steady state solution, it can take hours or even days for a problem to solve.

- String electric fields, which result in the plasma sheath, can lead to very high Peclet numbers. This means that the numerical scheme can become unstable unless the mesh is sufficiently fine in the plasma sheath.

- The external circuit connecting a CCP reactor to a power supply nearly always needs to be included in the model.

- Sharp geometric corners lead to substantial local electric fields that can result in nonphysical ion fluxes.

When the Electric Potential feature is active, it is possible to include quick options for the most common types of electrical circuit. The Circuit type has the following options, which affect the value of the electric potential imposed on the electrode. When the Circuit type is anything other than None, the electric potential imposed on the electrode, \( V \) is not necessary equal to the user supplied voltage, \( V_0 \).

<table>
<thead>
<tr>
<th>Circuit type</th>
<th>The Electrostatics Interface</th>
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</thead>
</table>

**NONE**

When the circuit type is set to None, the electric potential imposed at the electrode is equal to the user supplied electric potential:

\[
V = V_0.
\]
**Ballast Resistor**

This option places a ballast resistor between the user supplied electric potential and the applied voltage. In this case, the imposed value of the electric potential on the electrode becomes:

\[ V = V_0 - I_p R_b \]

where \( R_b \) is the value of the ballast resistor, and \( I_p \) is the total current flowing into the electrode. The current is computed by integrating the normal component of the electron and ion current densities over the electrode surface. This boundary condition should be used to prevent arcing in a DC discharge. If the plasma current becomes high, the magnitude of the applied voltage is reduced, thus avoiding a positive feedback loop where the plasma densities become extremely high.

**Series RC Circuit**

This option places a ballast resistor and blocking capacitor between the user supplied electric potential and the applied voltage. In steady state, this has the same effect as the ballast resistor option. One advantage of this option is that the imposed voltage on the electrode is smoothly ramped up from 0 to the setpoint in a time constant determined by the value of the ballast resistor and blocking capacitor. This can help with convergence when solving because it results in initial conditions which are consistent with the boundary conditions. The imposed value of the electric potential on the electrode becomes:

\[ V = V_0 - I_p R_b - R_b C_b \frac{dV}{dt} \]

This option is the preferred option to use when modeling DC discharges.

**Blocking Capacitor**

Another less useful option is to include a blocking capacitor in between the electrode and voltage source. In this case, the imposed value of the electric potential is given by the equation:

\[ C_b \frac{d}{dt} (V_0 - V) = I_p \]

where \( I_p \) is the current due to motion of charged carriers and the displacement current.
Theory for the DC Discharge Interface

The DC Discharge Interface theory is described in this section:

- Introduction to DC Discharge Theory
- DC Discharge Interface Boundary Conditions
- Tips for Modeling DC Discharges

Introduction to DC Discharge Theory

Due to the complexity of coupling the electrostatic field to the transport of electrons and heavy species, the Plasma Module provides this multiphysics interface specially designed for DC discharges. The complicated coupling between the electron transport, heavy species transport, and electrostatic field is handled automatically by the software. Furthermore, the secondary emission flux from ion bombardment on an electrode is automatically computed and used in the boundary condition for electrons. This makes it easy to model things such as positive columns and DC glow discharges.

The physics of DC discharges can be further complicated when a strong, static magnetic field is present. This can lead to highly anisotropic transport properties for the electrons. The DC Discharge interface automatically computes the tensor form of the electron mobility if requested. This makes it possible to model things such as magnetron discharges and hall thrusters. DC discharges require reaction rates to be specified in terms of Townsend rather than rate coefficients. The main reason is that Townsend coefficients provide a better description of the physics in the cathode fall region. The discharge is sustained by secondary emission, rather than a time varying electric field. Therefore, secondary emission effects must be included in any DC discharge model otherwise the plasma simply self extinguishes.

It is important to be aware of the different time scales at which the components of a plasma can change:

<table>
<thead>
<tr>
<th>PHENOMENA</th>
<th>TIME SCALE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetic field propagation</td>
<td>Instantaneous</td>
</tr>
<tr>
<td>Electron energy</td>
<td>&lt; 1 ns</td>
</tr>
</tbody>
</table>
DC Discharge Interface Boundary Conditions

Since secondary emission effects are vital in sustaining DC discharges, the boundary conditions play an important role in DC discharges. The secondary emission flux for electrons is defined as:

\[
\mathbf{n} \cdot \Gamma_{e,s} = \sum_{k=1}^{N} \gamma_k (\Gamma_k \cdot \mathbf{n})
\]

Additionally, the secondary emission energy flux requires that the mean energy of the secondary electrons are specified:

\[
\mathbf{n} \cdot \Gamma_{e,s} = \sum_{k=1}^{N} \gamma_k \tilde{\varepsilon}_k (\Gamma_k \cdot \mathbf{n})
\]

The secondary emission fluxes are automatically computed by the DC Discharge interface when surface reactions are added to a model. The mean electron energy of the emitted electrons, \( \tilde{\varepsilon}_k \), is typically a function of the ionization energy of the impinging ion and the work function of the surface:

\[
\tilde{\varepsilon}_k = \Delta \varepsilon_k - 2W_f
\]

where \( \Delta \varepsilon_k \) is the ionization energy (SI unit: eV) and \( W_f \) is the work function of the surface (SI unit: eV). On dielectric surfaces, charge accumulates due to the difference in fluxes between the electrons and ions:

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

where \( \mathbf{J}_i \) is the normal total ion current and \( \mathbf{J}_e \) is the normal total electron current. The surface charge density, \( \rho_s \), is used as a boundary condition in the Electrostatics interface.
CHAPTER 8: THE PLASMA REACTOR INTERFACES

Tips for Modeling DC Discharges

There are a number of key points to consider when modeling DC discharges:

• For atmospheric pressure DC discharges, the plasma might naturally try to arc. This typically causes the solver to terminate because it can’t reach the desired tolerances. Often this behavior is undesired, so in practical experimental setups a series RC circuit is added between the driven electrode and the power supply. This prevents arcing from occurring and results in a glow discharge. It is recommended to use the Series RC circuit option in the Circuit Settings section of the Electric Potential feature.

• Townsend coefficients should be used in preference to rate coefficients if possible. Townsend coefficients give a more realistic description of cathode fall regions in DC discharges. It is only possible to use Townsend coefficients when the Formulation property is set to Finite element.

• Secondary emission from a surface bombarded by ions must be included somewhere in the model in order for the discharge to be sustained.

• Although a DC discharge ultimately reaches a steady state condition, the problem must be solved as a time-dependent problem so the plasma can naturally evolve into its equilibrium state.

• The initial conditions should enforce the electroneutrality constraint.

\[-\mathbf{n} \cdot \mathbf{D} = \rho_s\]
Theory for the Inductively Coupled and Microwave Plasma Interfaces

The Inductively Coupled Plasma Interface and The Microwave Plasma Interface theory is described in this section:

- Introduction to Inductively Coupled Plasmas
- Domain Equations for the Inductively Coupled Plasma Interface
- Wave Heated Discharge Theory
- Domain Equations for the Microwave Plasma Interface
- Plasma Conductivity in the Presence of a Static Magnetic Field

Introduction to Inductively Coupled Plasmas

Inductively coupled plasma (ICP) reactors are important in plasma processing and plasma sources because the plasma density can be considerably higher than in capacitively coupled discharges. ICP reactors are also attractive from the modeling perspective because they are relatively straightforward to model. Inductively coupled plasmas are relatively straightforward to model due to the fact that the induction currents can be solved for in the frequency domain. This means that the RF cycle applied to the driving coil does not need to be explicitly resolved. As such, the quasi steady-state solution is reached in relatively few time steps.

In a 2D axial symmetric ICP reactor, a coil driven at a high frequency (usually 13.56 MHz) creates a magnetic field with only an in-plane component (the r-z plane) and a high frequency out-of-plane component of the electric field (in the \( \theta \)-direction). This results in oscillatory electron motion in the \( \theta \)-direction only. Due to this effect, further simplifications can be made and the out-of-plane electric field can be solved for in the frequency domain. Consider the momentum conservation of electrons as given in Equation 6-3:

\[
\frac{\partial}{\partial t}(n_e m_e \mathbf{u}_e) + \nabla \cdot n_e m_e \mathbf{u}_e \mathbf{u}_e^T = - \nabla \cdot \mathbf{p}_e + q n_e \mathbf{E} - n_e m_e \mathbf{u}_e \mathbf{v}_m
\]

where \( m_e \) is the electron mass (SI unit: kg), \( \mathbf{u}_e \) is the drift velocity of the electrons (SI unit: m/s), \( \mathbf{p}_e \) is the electron pressure tensor (SI unit: Pa), \( q \) is the electron charge (SI unit: s A), \( \mathbf{E} \) is the electric field (SI unit: V/m) and \( \mathbf{v}_m \) is the momentum transfer.
frequency (SI unit: 1/s). Neglecting the inertial term and taking only the \( \theta \)-component yields:

\[
\frac{\partial}{\partial t}(n_e m_e u_{e, \theta}) = -\frac{e}{Z_0} (n_e k_B T_e) + q n_e E_0 - n_e m_e u_{e, \theta} \nu_m.
\]

Since \( n_e \) and \( T_e \) are uniform in the \( \theta \)-direction, the first term on the right and side can be neglected, resulting in:

\[
\frac{\partial}{\partial t}(n_e m_e u_{e, \theta}) = q n_e E_0 - n_e m_e u_{e, \theta} \nu_m
\]

which is a linear equation in \( u_{e, \theta} \) which can be Fourier transformed by letting:

\[
E_0 = \hat{E}_0 e^{j\omega t}
\]

and

\[
u_{e, \theta} = \hat{u}_{e, \theta} e^{j\omega t}
\]

the resulting equation in the frequency domain is:

\[
-j\omega n_e m_e \hat{u}_{e, \theta} = q n_e \hat{E}_0 - n_e m_e \hat{u}_{e, \theta} \nu_m.
\]

Multiplying this equation by \( q \) and defining the out-of-plane electron current density as:

\[
\hat{J}_0 = q n_e \hat{u}_{e, \theta}
\]

the following expression is obtained:

\[
\hat{J}_0 = \frac{q^2 n_e}{m_e (\nu_m + j\omega)} \hat{E}_0
\]

which relates the current density to the electric field in the form of \( J_0 = \sigma E_0 \) with the plasma conductivity, \( \sigma \) defined as:

\[
\sigma = \frac{q^2 n_e}{m_e (\nu_m + j\omega)}
\]

which is required by Equation 8-4. The third term on the left hand side of Equation 6-4 now has an additional contribution due to the out-of-plane motion of the electrons.
The presence of the driving coil in an ICP reactor also introduces capacitive coupling between the coil and the electrons in the plasma sheath. This is neglected in COMSOL Multiphysics. This is because the electron density in an ICP reactor is typically so high that the Debye length is very small, meaning that the in-plane component of the electric field cannot penetrate into the plasma.

When collisionless heating is included in the model an extra degree of freedom for the out-of-plane electron drift velocity is added:

\[ n_e u_{\phi} \text{Re} + n_e v_e u_{\phi} - \eta_{\text{eff}} \nabla \cdot (n_e \nabla u_{\phi}) = \frac{e}{m_e} n_e E_{\phi} \]

where \( \eta_{\text{eff}} \) is the effective viscosity coefficient defined as:

\[ \eta_{\text{eff}} = \left( \frac{e^2 V_{th}^2}{\pi^2 \omega_p \omega} \right)^{1/3} \]

and \( V_{th} \) is the thermal velocity defined as:

\[ V_{th} = \left( \frac{3T_e}{m_e} \right)^{1/2} \]

and \( \omega_p \) is the plasma frequency defined as:

\[ \omega_p = \left( \frac{e^2 n_e}{\epsilon_0 m_e} \right)^{1/2} \]

The plasma conductivity, \( \sigma \), is set to zero and the out-of-plane current density, \( J_{\phi} \) has the following term added to it:

\[ J_{\phi} = n_e u_{\phi} q \]

**Domain Equations for the Inductively Coupled Plasma Interface**

The Inductively Coupled Plasma Interface solves a system of coupled partial differential equations for:

- The electron density
• The mean electron energy
• The mass fraction of each of the heavy species
• The electrostatic potential
• The electric field due to induction currents

For a nonpolarized plasma, the induction currents are computed in the frequency domain using the following equation:

\[(j\omega \sigma_0 - \omega^2 \varepsilon_0 \varepsilon_r) A + \nabla \times (\mu_0^{-1} \nabla \times A) = J^p \quad (8-4)\]

---

**Wave Heated Discharge Theory**

Wave heated discharges usually fall into one of two categories, discharges with no external DC magnetic field, and discharges with a high intensity static magnetic field.

If a suitably high DC magnetic field is present then electron cyclotron resonance (ECR) can occur where electrons continually gain energy from the electric field over 1 RF period. Modeling microwave plasmas involves solving equations for the electron density, mean electron energy, heavy species, the electrostatic potential, and the high frequency electric field. The high frequency electric field is computed in the frequency domain and losses are introduced via a complex plasma conductivity.

The derivation of the expression for the plasma conductivity occurs in the same manner as for the ICP from the momentum conservation equation. The motion of the
electrons in a microwave plasma occurs mainly due to the ambipolar field and diffusion in the plasma sheath.

In COMSOL Multiphysics the absorption of electromagnetic waves must be realized through a complex electrical conductivity. It is not possible to specify a complex permittivity. The microwave plasma interface automatically computes the plasma conductivity based on the electron density, collision frequency and any external DC magnetic flux density that is present.

**Domain Equations for the Microwave Plasma Interface**

The wave heated discharge solves a system of coupled partial differential equations. In a microwave reactor the high frequency electric field is computed in the frequency domain using the following equation:

\[
\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k_0^2 \left( \varepsilon_r - \frac{j\sigma}{\varepsilon_0} \right) \mathbf{E} = 0
\]

(8-5)

**Plasma Conductivity in the Presence of a Static Magnetic Field**

The relationship between the plasma current density and the electric field becomes more complicated in the presence of a DC magnetic field. The following equation defines this relationship:

\[
\sigma^{-1} \mathbf{J} = \mathbf{E}
\]
where $\sigma$ is the plasma conductivity tensor which is a function of the electron density, collision frequency and magnetic flux density. Using the definitions:

$$\alpha = \frac{q}{m_e (v_e + j\omega)}$$

$$\beta = n_e q \alpha$$

where $q$ is the electron charge, $m_e$ is the electron mass, $n_e$ is the collision frequency, and $\omega$ is the angular frequency of the electromagnetic field, the inverse of the plasma conductivity can be written as:

$$\sigma^{-1} = \begin{bmatrix}
\frac{1}{\beta} & -\frac{\alpha B_z}{\beta} & \frac{\alpha B_y}{\beta} \\
-\frac{\alpha B_z}{\beta} & \frac{1}{\beta} & -\frac{\alpha B_x}{\beta} \\
\frac{\alpha B_y}{\beta} & \frac{\alpha B_x}{\beta} & \frac{1}{\beta}
\end{bmatrix}$$

where $B$ is the magnetic flux density which has three components $B_x, B_y,$ and $B_z$. The inverse of the plasma conductivity is used because it can be written in a compact, convenient form. The plasma conductivity is a highly nonlinear function of the magnetic flux density. The conductivity exhibits resonant behavior at a critical magnetic flux density given by the simple formula:

$$B_{res} = \frac{m_e \omega}{q}$$

At this critical magnetic flux density the electrons continually gain energy from the electric field at all phases of the RF cycle. This principle, called electron cyclotron resonance is exploited in ECR reactors.
Index

2D axisymmetric models
laminar flow and 125

A
absolute pressure 102
activation energy 205
advanced settings 18
Arrhenius coefficients
data requirements 27
Arrhenius expressions 204, 226
Arrhenius parameters 203

B
Babuska-Brezzi condition 144
base node 69
Basset history term 150
Boltzmann equation, two-term approximation interface 154
theory 163
Boltzmann model (node) 158
boundary conditions
inlet and outlet, theory 132
boundary nodes
Boltzmann equation, two-term approximation 157, 161
capacitively coupled plasma interface 238
drift diffusion 174
electrostatics 38
heavy species transport 198
inductively coupled plasma interface 248
microwave plasma interface 258
single-phase flow 101
boundary selection 19
boundary stress (node) 115
Boussinesq approximation 128
bulk node 70

C
capacitively coupled plasma interface 232

theory 264
capacitor (node) 63
CFL number
settings 99
theory 148
change cross-section (node) 58
change thickness (out-of-plane) (node) 59
charge conservation (node) 40
charge relaxation theory 75
circuit import, SPICE 73
closure law 219
collector node 69
collision (node) 160
collisionless heating (node) 254
compressible flow 127
consistent stabilization
settings 18
constraint settings 18
continuity on interior boundary (node) 243
coupling, to the electrical circuits interface 91
cross section import (node) 199
cross-section data
electron impact reactions, and 26
importing 30
crosswind diffusion
fluid flow 143
current source (node) 65
current sources, theory 77
current-controlled current source (node) 67
current-controlled voltage source (node) 67
D  data requirements 26
   DC discharge interface 244
      theory 266
   DC magnetic field 233
   device models, electrical circuits 81
   dielectric shielding (node) 50
   diffusion and migration (node) 199
   diffusion models 194, 233
   diffusive flux vector 216
   diode (node) 70
   diode transistor model 86
   discharges, non-equilibrium 12
   discontinuous Galerkin
      fluid flow 149
   discretization 18
   distributed capacitance (node) 54
   distribution functions 164
   documentation 20
   domain nodes
      Boltzmann equation, two-term approximation 157
      capacitively coupled plasma interface 238
      drift diffusion 174
      electrostatics 38
      heavy species transport 198
      inductively coupled plasma interface 248
      microwave plasma interface 258
      single-phase flow 101
   domain selection 19
   double dot product 124
   drain node 70
   drift diffusion interface 172
      theory 184
   drift diffusion model (node) 175
   drift velocity 167
   drift velocity, calculating 163
Druyvesteyn distribution function 164
Druyvesteyn EEDF 196, 235
E  edge nodes
      capacitively coupled plasma interface 238
      electrostatics 38
      microwave plasma interface 258
   edge selection 19
   EEDF 163
   Einstein’s relation 208, 217
   elastic collisions, data requirements 27
   electric displacement field (node) 47
   electric fields theory 75
   electric potential (node) 44
   electrical circuit interface 61
      theory 80
   electrical circuits
      modeling techniques 90
      electron cyclotron resonance (ECR) 272
      electron density and energy (node) 180
      electron energy distribution function 163
      electron impact reaction (node) 200
      electron impact reactions, data requirements and 26
   electron outlet (node) 183
   electron production rate (node) 178
   electron-electron collisions 165
   electrostatic point dipole (node) 59
   electrostatics interface 36
      theory 78
   emailing COMSOL 22
   emission energy and fluxes 267
   emitter node 69
   enthalpy and entropy 220
   equation of continuity 75
   equation view 18
   error message, electrical circuits 90
   exit length 113
<table>
<thead>
<tr>
<th>Index</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>floating potential (node)</td>
</tr>
<tr>
<td></td>
<td>electrostatics 52</td>
</tr>
<tr>
<td></td>
<td>flow continuity (node) 119</td>
</tr>
<tr>
<td></td>
<td>flow rate in SCCMs 111</td>
</tr>
<tr>
<td></td>
<td>fluid flow</td>
</tr>
<tr>
<td></td>
<td>Mach number 126</td>
</tr>
<tr>
<td></td>
<td>particle tracing 149</td>
</tr>
<tr>
<td></td>
<td>single-phase theory 123</td>
</tr>
<tr>
<td></td>
<td>flux (node)</td>
</tr>
<tr>
<td></td>
<td>drift diffusion 183</td>
</tr>
<tr>
<td></td>
<td>heavy species transport 212</td>
</tr>
<tr>
<td></td>
<td>forward rate constants 27</td>
</tr>
<tr>
<td></td>
<td>forward sticking coefficients 27</td>
</tr>
<tr>
<td></td>
<td>frequency factor 205</td>
</tr>
<tr>
<td></td>
<td>frequency factor for reaction 220</td>
</tr>
<tr>
<td>G</td>
<td>Galerkin formulation, fluid flow 149</td>
</tr>
<tr>
<td></td>
<td>Galerkin least-squares (GLS), stabilization 143</td>
</tr>
<tr>
<td></td>
<td>gas constant 205</td>
</tr>
<tr>
<td></td>
<td>gas phase reactions 27</td>
</tr>
<tr>
<td></td>
<td>gas phase solvent 223</td>
</tr>
<tr>
<td></td>
<td>gate node 70</td>
</tr>
<tr>
<td></td>
<td>gauge fixing for A-field (node) 255</td>
</tr>
<tr>
<td></td>
<td>Gauss’ law and charge relaxation theory 75</td>
</tr>
<tr>
<td></td>
<td>Gauss’ law equation 78</td>
</tr>
<tr>
<td></td>
<td>general power deposition (node) 179</td>
</tr>
<tr>
<td></td>
<td>general stress (boundary stress condition) 115</td>
</tr>
<tr>
<td></td>
<td>generalized distribution function 164</td>
</tr>
<tr>
<td></td>
<td>geometric entity selection 19</td>
</tr>
<tr>
<td></td>
<td>ground (node) 43</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Character</td>
<td>Description</td>
</tr>
<tr>
<td>-----------</td>
<td>-------------</td>
</tr>
<tr>
<td>ion</td>
<td>flux 264</td>
</tr>
<tr>
<td>isotropic</td>
<td>diffusion</td>
</tr>
<tr>
<td>fluid</td>
<td>flow 143</td>
</tr>
<tr>
<td>K</td>
<td>Khan-Richardson model 149</td>
</tr>
<tr>
<td></td>
<td>kinetic gas theory 221</td>
</tr>
<tr>
<td></td>
<td>Kirchhoff's circuit laws 80</td>
</tr>
<tr>
<td></td>
<td>knowledge base, COMSOL 22</td>
</tr>
<tr>
<td>L</td>
<td>laminar flow</td>
</tr>
<tr>
<td></td>
<td>Reynolds number, and 127</td>
</tr>
<tr>
<td></td>
<td>laminar flow interface 98</td>
</tr>
<tr>
<td></td>
<td>theory 123</td>
</tr>
<tr>
<td></td>
<td>laminar inflow (inlet boundary condition) 108</td>
</tr>
<tr>
<td></td>
<td>laminar outflow (outlet boundary condition) 112</td>
</tr>
<tr>
<td></td>
<td>law of mass action 225</td>
</tr>
<tr>
<td></td>
<td>leaking wall, wall boundary condition 106</td>
</tr>
<tr>
<td></td>
<td>line charge (node) 54</td>
</tr>
<tr>
<td></td>
<td>line charge (on axis) (node) 55</td>
</tr>
<tr>
<td></td>
<td>line charge (out-of-plane) (node) 56</td>
</tr>
<tr>
<td></td>
<td>line mass source (node)</td>
</tr>
<tr>
<td></td>
<td>fluid flow 120</td>
</tr>
<tr>
<td></td>
<td>line source</td>
</tr>
<tr>
<td></td>
<td>fluid flow 142</td>
</tr>
<tr>
<td></td>
<td>local</td>
</tr>
<tr>
<td></td>
<td>CFL number 99, 148</td>
</tr>
<tr>
<td></td>
<td>low-temperature plasmas 12</td>
</tr>
<tr>
<td></td>
<td>lumped curves 139</td>
</tr>
<tr>
<td>M</td>
<td>Mach number</td>
</tr>
<tr>
<td></td>
<td>definition, single-phase flow 126</td>
</tr>
<tr>
<td></td>
<td>mass flow inlet, theory 135</td>
</tr>
<tr>
<td></td>
<td>mass flow rate, theory 135</td>
</tr>
<tr>
<td></td>
<td>mass sources</td>
</tr>
<tr>
<td></td>
<td>fluid flow 141</td>
</tr>
<tr>
<td></td>
<td>Maxwell's equations</td>
</tr>
<tr>
<td></td>
<td>electrical circuits and 80</td>
</tr>
<tr>
<td></td>
<td>Maxwellian distribution function 164</td>
</tr>
<tr>
<td></td>
<td>Maxwellian EEDF 189, 195, 234</td>
</tr>
<tr>
<td></td>
<td>Maxwell-Stefan equations 215</td>
</tr>
<tr>
<td></td>
<td>microwave plasma interface 256</td>
</tr>
<tr>
<td></td>
<td>theory 269, 272</td>
</tr>
<tr>
<td></td>
<td>microwave power deposition (node) 180</td>
</tr>
<tr>
<td></td>
<td>Model Libraries window 21</td>
</tr>
<tr>
<td></td>
<td>model library examples</td>
</tr>
<tr>
<td></td>
<td>Boltzmann models 157</td>
</tr>
<tr>
<td></td>
<td>CCP models 238</td>
</tr>
<tr>
<td></td>
<td>DC models 245</td>
</tr>
<tr>
<td></td>
<td>drift diffusion 174</td>
</tr>
<tr>
<td></td>
<td>electrical circuits 90</td>
</tr>
<tr>
<td></td>
<td>electrostatics 37</td>
</tr>
<tr>
<td></td>
<td>flux matching 227</td>
</tr>
<tr>
<td></td>
<td>heavy species transport 197</td>
</tr>
<tr>
<td></td>
<td>ICP models 248</td>
</tr>
<tr>
<td></td>
<td>laminar flow 101</td>
</tr>
<tr>
<td></td>
<td>microwave plasmas 258</td>
</tr>
<tr>
<td></td>
<td>modeling plasmas 12</td>
</tr>
<tr>
<td></td>
<td>molar enthalpy and entropy 220</td>
</tr>
<tr>
<td></td>
<td>Motz-Wise correction 210</td>
</tr>
<tr>
<td></td>
<td>moving wall, wall boundary condition 106</td>
</tr>
<tr>
<td></td>
<td>MPH-files 21</td>
</tr>
<tr>
<td></td>
<td>multicomponent diffusion 216</td>
</tr>
<tr>
<td></td>
<td>multicomponent mixtures 223</td>
</tr>
<tr>
<td>N</td>
<td>NASA polynomials 28, 220</td>
</tr>
<tr>
<td></td>
<td>Navier-Stokes equations 124</td>
</tr>
<tr>
<td></td>
<td>n-Channel MOS transistor 69, 83</td>
</tr>
<tr>
<td></td>
<td>n-Channel MOSFET (node) 69</td>
</tr>
<tr>
<td></td>
<td>netlists, SPICE 73, 94</td>
</tr>
<tr>
<td></td>
<td>neutral gas temperature 28</td>
</tr>
<tr>
<td></td>
<td>niterCMP variable 148</td>
</tr>
<tr>
<td></td>
<td>no slip, wall boundary condition 105</td>
</tr>
<tr>
<td></td>
<td>no viscous stress (open boundary) 114</td>
</tr>
<tr>
<td></td>
<td>nomenclature, in the Plasma Module 14</td>
</tr>
<tr>
<td></td>
<td>non-electron species 263</td>
</tr>
<tr>
<td></td>
<td>non-equilibrium discharges 12</td>
</tr>
<tr>
<td></td>
<td>non-Newtonian fluids 125</td>
</tr>
</tbody>
</table>
INDEX

P

pair nodes
Boltzmann equation, two-term approximation 157
capacitively coupled plasma interface 238

drift diffusion 174
electrostatics 38
heavy species transport 198
inductively coupled plasma interface 248
microwave plasma interface 258
single-phase flow 101
pair selection 19
particle tracing in fluid flow 149
Peclet numbers 264
periodic condition (node) 48
periodic flow condition (node) 118
plasma model (node)
capacitively coupled plasma interface 239
inductively coupled plasma interface 251
plasma reactor theory 261
point charge (node) 56
point charge (on axis) (node) 57
point mass source (node)
fluid flow 119
point nodes
capacitively coupled plasma interface 238
electrostatics 38
inductively coupled plasma interface 248
microwave plasma interface 258
single-phase flow 101
point selection 19
point source
fluid flow 141
pointwise mass flux, theory 135
Poisson’s equation 14
predefined couplings, electrical circuits 91
pressure (outlet boundary condition) 112
pressure point constraint (node) 121
pressure, no viscous stress (inlet and outlet boundary conditions) 108
pseudo time stepping
laminar flow theory 147
settings 99
theory 148

R
rate expression for species 216
reaction (node) 204
reaction rate 220
reflection coefficient 190
resistor (node) 63
Reynolds number definition 127
Reynolds particle number 150
RF cycle 264, 269

S
SCCM, flow rate in 111
SEMI standard E12-0303 110
semiconductor device models 81

normal stress (boundary condition) 108
normal stress, normal flow (boundary stress condition) 116
NPN bipolar junction transistor 69, 81
NPN BJT (node) 69

O
Ohm’s law and charge relaxation theory 75
open boundary (node)
single-phase flow 114
outflow (node) 213
outlet (node) 111
outlet boundary condition 139
outlet boundary condition, theory 132
override and contribution 18

NPN bipolar junction transistor 69, 81
NPN BJT (node) 69
settings windows 18
shear rate magnitude variable 103
show (button) 18
single-phase flow interface
  laminar flow 98
  theory 123
SIPG method 149
sliding wall, wall boundary condition 105
  theory 130
slip velocity, wall boundary condition 106
  theory 130
slip, wall boundary condition 105
  theory 129
source coefficients 188, 262
source node 70
space charge density (node) 42
species (node) 205
species dipole moment 223
spf.cellRe variable 128
spf.sr variable 103
SPICE netlists 13, 73, 94
stabilization settings 18
standard cubic centimeters per minute
  111
standard flow rate 111
standard flow rate, theory 136
static pressure curves 116
steady state condition 268
sticking coefficients 226
Stiel-Thodos equation 223
stoichiometric coefficients 225
stoichiometric matrix 220
streamline diffusion
  fluid flow 143
subcircuit definition (node) 68
subcircuit instance (node) 68
surface charge accumulation (node) 49
  surface charge density (node) 46
  surface reaction (node) 209
  surface reactions 27
  surface reactions, theory 225
  surface species (node) 211
  symmetric interior penalty Galerkin
    method (SIPG) 149
  symmetry (node) 113
TE mode 257
technical support, COMSOL 22
TEM mode 257
temperature exponent 205
temperatures, ranges for 208
terminal (node)
  electrostatics 51
  theory
    Boltzmann equation, two-term approximation 163
    capacitively coupled plasma interface 264
    DC discharges interface 266
drift diffusion 184
electric fields 75
electrical circuit interface 80
electrostatics interface 78
heavy species transport 215
inductively coupled plasma interface 269
inlet and outlet boundary conditions 132
laminar flow 123
microwave plasma interface 269, 272
plasma reactors 261
single-phase flow 123
  source coefficients 188, 262
thermal conductivity 223
thermal creep, wall boundary condition 106
thermionic emission 175
thermodynamic polynomials 208
thermophoretic effects 207
thin low permittivity gap (node) 49
TM mode 257
Townsend coefficients 168
Townsend coefficients theory 188, 262
traction boundary conditions 115

U  user community, COMSOL 22

V  vacuum pump (node) 116
vacuum pump theory 139
variables
  niterCMP 148
  spf.cellRe 128
velocity (inlet and outlet boundary conditions) 108
velocity (node) 179
viscous slip, wall boundary condition 106
viscous stress, theory 136
voltage source (node) 64
voltage-controlled current source (node) 66
voltage-controlled voltage source (node) 66
volume force (node) 103

W  wall (node)
  drift diffusion 181
  single-phase flow 104
  wave heated discharge 273
  weak constraint settings 18
  weakly ionized 186
  web sites, COMSOL 22

Z  zero charge (node) 42
zero energy flux (node) 162
zero probability (node) 162