INTRODUCTION TO

Plasma Module

COMSOL

Introduction to the Plasma Module

Version: COMSOL 5.5

Contact Information

Visit the Contact COMSOL page at www.comsol.com/contact to submit general inquiries, contact Technical Support, or search for an address and phone number. You can also visit the Worldwide Sales Offices page at www.comsol.com/contact/offices for address and contact information.

If you need to contact Support, an online request form is located at the COMSOL Access page at www.comsol.com/support/case. Other useful links include:

- Support Center: www.comsol.com/support
- Product Download: www.comsol.com/product-download
- Product Updates: www.comsol.com/support/updates
- COMSOL Blog: www.comsol.com/blogs
- Discussion Forum: www.comsol.com/community
- Events: www.comsol.com/events
- COMSOL Video Gallery: www.comsol.com/video
- Support Knowledge Base: www.comsol.com/support/knowledgebase

Contents

Introduction

The Plasma Module is tailor-made to model and simulate low-temperature plasma sources and systems. Engineers and scientists use it to gain insight into the physics of discharges and gauge the performance of existing or potential designs. The module can perform analysis in all space dimensions — 1D, 2D, and 3D — although it is very rare in the plasma modeling community to do 3D modeling. Plasma systems are, by their very nature, complicated systems with a high degree of nonlinearity. Small changes to the electrical input or plasma chemistry can result in significant changes in the discharge characteristics.

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 and equilibrium discharges, which occur in a wide range of engineering disciplines.

The Plasma Module consists of a suite of physics interfaces that allow arbitrary systems to be modeled, a set of documented examples, and a manual. The intended audience is researchers and engineers with a background in the physics of low-temperature discharges.

Applications of Plasmas in Science & Technology

There are many different types of plasma that are typically of interest. The main difference between the plasmas is that the mechanism of energy transfer between the electrons and fields is different. In this section the following types of plasma are discussed:

- Direct Current Discharges
- Inductively coupled plasmas
- Capacitively Coupled Plasmas
- Microwave Plasmas
- Plasma-enhanced Chemical Vapor Deposition
- Dielectric Barrier Discharges
- Space Thrusters and Magnetron Sputtering
- Equilibrium Discharges

DIRECT CURRENT DISCHARGES

Direct current (DC) discharges are sustained through secondary electron emission at the cathode due to ion bombardment. The electrons ejected from the cathode are accelerated through the cathode fall region into the bulk of the plasma. They

may acquire enough energy to ionize the background gas, creating a new electron-ion pair. The electron makes its way to the anode whereas the ion will migrate to the cathode, where it may create a new secondary electron. It is not possible to sustain a DC discharge without including secondary electron emission.

Several distinct regions typically exist in a DC discharge, depending on the specific operating conditions and geometry. A typically DC discharge is shown below. The cathode glow (often known as *cathode fall*) region is where most of the voltage drop occurs. This is the region where the discharge current is built up due to the high degree of ionization. The electron density and flux grow exponentially in this region (Ref. 5). The negative glow and Faraday space regions connect the cathode glow to the positive column. In this region the electron temperature drops rapidly due to the fact that the electric field is very weak. In the positive column region, the discharge is very uniform, and the electron-ion pairs generated are lost to the walls in the radial direction due to the ambipolar field (Ref. 5).
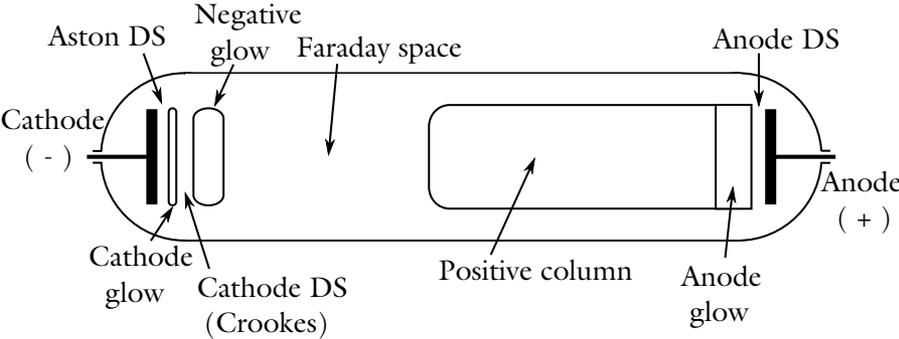

Diagram showing the most important regions in a typical DC discharge, after Ref. 5.

DC discharges can easily begin to arc, especially at high pressures. Arcing is typically undesirable so, in practice, a ballast resistor or series RC circuit is placed between the power supply and the cathode. As the discharge current at the cathode begins to increase, the voltage applied at the cathode will begin to drop due to the presence of the RC circuit. If the ballast resistance is high enough, the DC discharge will remain smooth and uniform and not begin to arc. The pressure range for a DC discharge is typically in the range of 10 Pa all the way up to

atmospheric pressure and the applied voltage is typically several hundred volts all the way up to several kV.
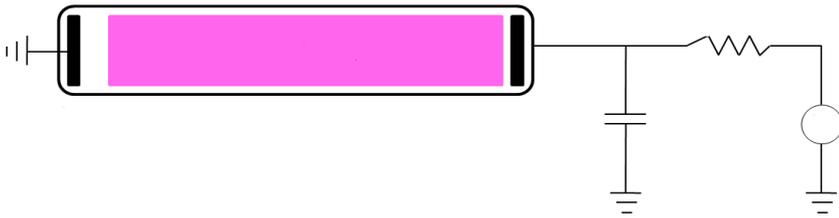

Schematic of a positive column DC discharge including an external circuit. The ballast resistor and blocking capacitor prevent the discharge from arcing.

INDUCTIVELY COUPLED PLASMAS

Inductively coupled plasmas (ICP) were first used in the 1960s as thermal plasmas in coating equipment, Ref. 4. These devices operated at pressures on the order of 0.1 atm and produced gas temperatures on the order of 10,000 K. In the 1990s, ICP became popular in the film processing industry as a way of fabricating large semiconductor wafers. These plasmas operated in the low-pressure regime, from 0.002–1 Torr and, as a consequence the gas temperature remained close to room temperature. Low-pressure ICP are attractive because they provide a relatively uniform plasma density over a large volume. The plasma density is also high, around 10^{18} $1/m^3$, which results in a significant ion flux to the surface of the wafer. Faraday shields are often added to reduce the effect of capacitive coupling between the plasma and the driving coil. This reduces the effect of ion bombardment on the dielectric window, which can lead to degradation and

contamination of the chamber. Some typical ICP configurations are shown in the figure below.
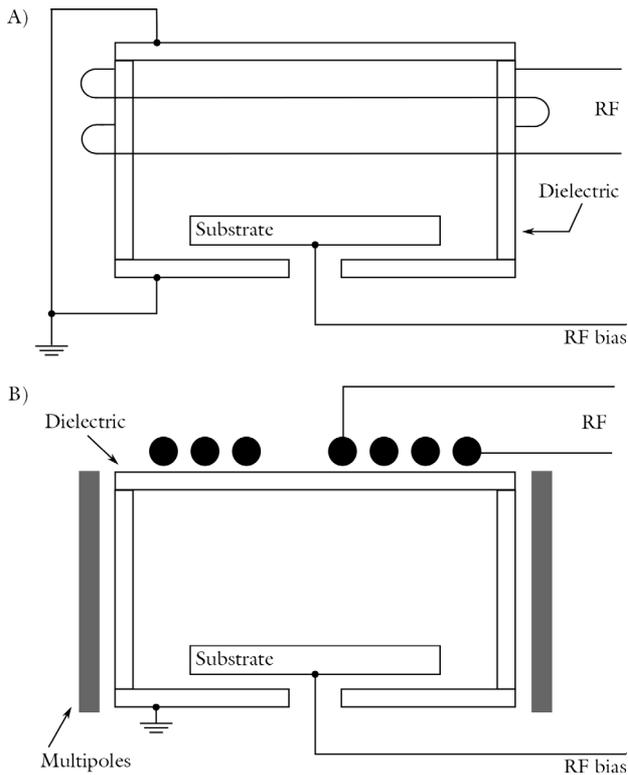
Sketch of some typical ICP configurations used in the semiconductor processing industry, after Ref. 5.

From an electrical point of view, inductively coupled plasmas act like transformers, with the driving coil acting as the primary and the plasma acting as the secondary. The current flowing through the coil induces a current in the plasma, causing the electrons to flow in the opposite direction to the current flowing in the coil. This, in turn, induces an opposing current back in the coil. The coil and plasma are strongly coupled. Heating of the electrons only occurs within the skin depth of the plasma. The higher the plasma density or the applied frequency, the smaller the volume over which power is deposited from the fields to the electrons. The design and operating frequency of the coil should be such that the plasma is

uniform over the reactor volume. Often this means the power should be as uniformly deposited within the plasma as possible.
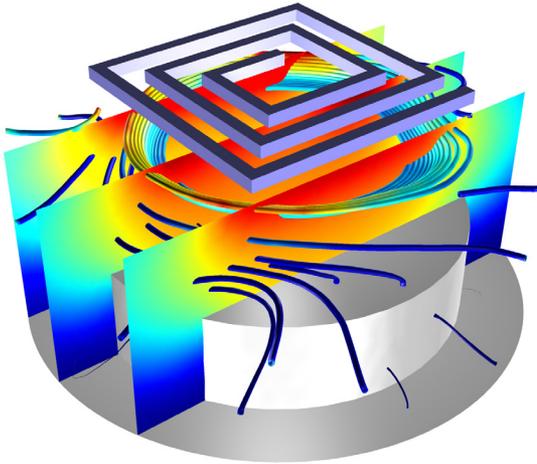
Inductively Coupled Plasma. The electron temperature is shown as a slice plot and the current density induced in the plasma is shown as streamlines. The plasma is created and sustained via a rectangular single spiral coil.

CAPACITIVELY COUPLED PLASMAS

Capacitively coupled plasmas (CCP) are often used in the semiconductor industry to deposit dielectric films on semiconductor wafers. A typical CCP configuration is shown to the right. Unlike a DC discharge, the electrodes are coated in a dielectric material, which becomes charged due to the accumulation of positive or negative charges. By driving the electrodes with a sinusoidal voltage, typically at frequencies ranging from 100 kHz up to 100 MHz, the discharge can sustain itself without requiring secondary electron emission (Ref. 4). This is because the electrons are very light, so they respond to the electric field, almost instantaneously. This allows for energy transfer from the fields to the
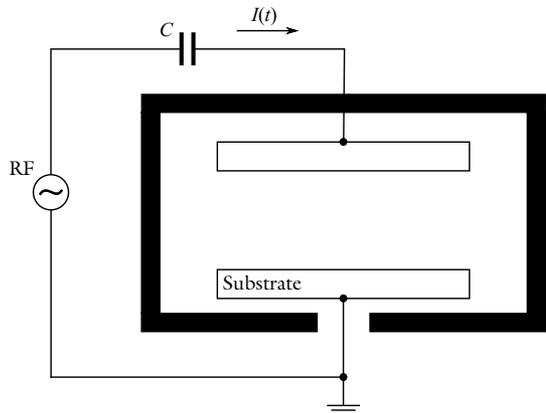
electrons which is responsible for sustaining the plasma. Ions are much more massive than the electrons, so they respond only to the time averaged electric field. The mechanism of power transfer from the fields to the electrons is a highly nonlinear process, occurring at frequencies other than simply twice the angular frequency.

Typical operating conditions for capacitively coupled plasmas are driving voltages from 100–1000 V, pressures of 2–200 Pa, electron densities in the region of 10^{15}–10^{17} $1/m^3$ and electron temperatures on the order of 2–20 eV. The operating frequency is typically 13.56 MHz, which is one of the frequencies reserved worldwide for the industrial, scientific, and medical uses.
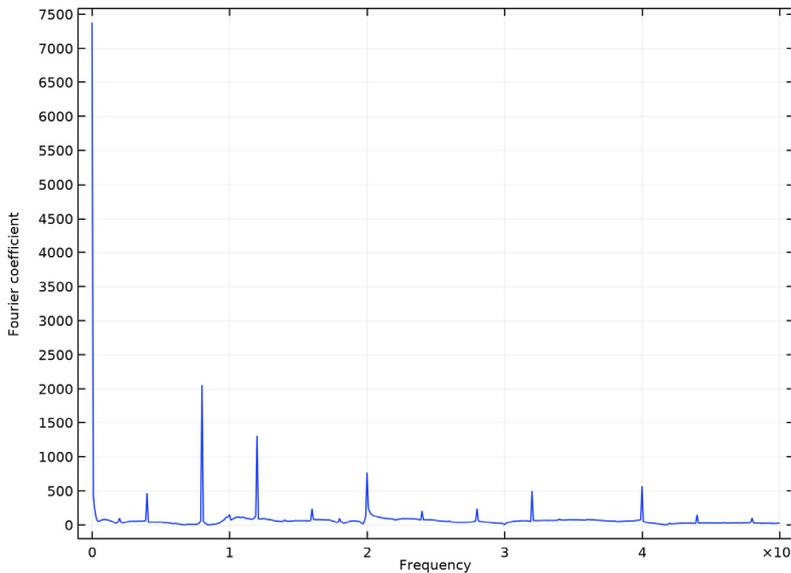
Frequency content of the power deposition into a dual frequency capacitively coupled plasma. The power deposition occurs at multiple different frequencies indicating a complex mechanism of power transfer from the fields to the electrons.

MICROWAVE PLASMAS

Microwave plasmas, or *wave heated discharges*, are sustained when electrons can gain enough energy from an electromagnetic wave as it penetrates into the plasma. The physics of a microwave plasma is quite different depending on whether the TE mode (out-of-plane electric field) or the TM mode (in-plane electric field) is propagating. In the 2D axisymmetric case, the TE mode means that only the azimuthal component of the electric field is computed and the TM mode means that the in-plane, r and z components of the electric field are computed. In both

cases it is not possible for the electromagnetic wave to penetrate into regions of the plasma where the electron density exceeds the critical electron density (around $7.6\mathrm{x}10^{16}$ $1/\mathrm{m}^3$ for argon at 2.45 GHz). On this contour corresponding to the critical electron density, the wave goes from being propagating to evanescent. This means that all the power from the wave is absorbed in a very small region in space, which can make the model numerically unstable. The pressure range for microwave plasmas is very broad. For electron cyclotron resonance (ECR) plasmas, the pressure can be on the order of 1 Pa or less. For non-ECR plasmas the pressure typically ranges from 100 Pa up to atmospheric pressure. The power can range from a few watts all the way up to several kilowatts. Microwave plasmas are popular due to the cheap availability of microwave power.
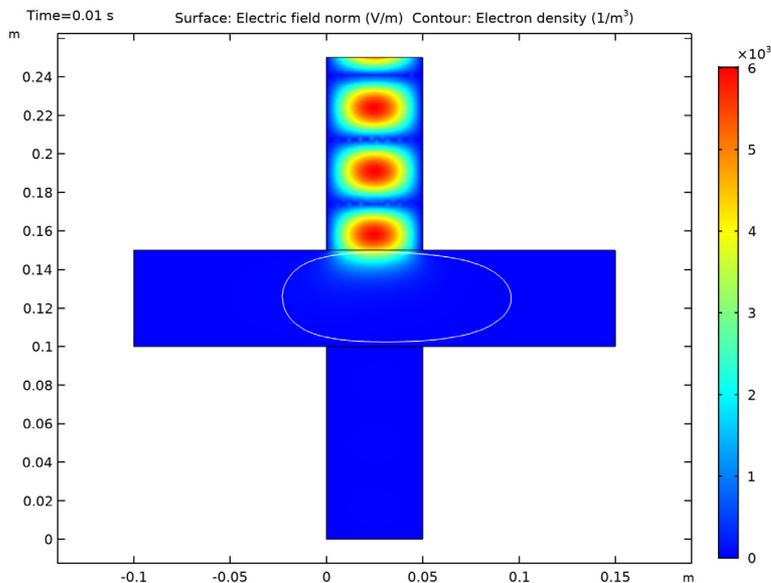
Electric field (surface) and critical electron density (white contour) in a cross-configuration microwave plasma.

PLASMA-ENHANCED CHEMICAL VAPOR DEPOSITION

Plasma-enhanced chemical vapor deposition (PECVD) is a discharge operating in a reactive gas. It is used as an alternative to traditional chemical vapor deposition, since it can generate the radical species required to initiate the deposition process very efficiently, without the need for very high gas temperatures. In the case of silicon deposition in a silane plasma, the electron impact reactions can dissociate the silane into highly reactive silicon hydrides and hydrogen gas. Equally as important as the gas phase reactions is the complicated set of chemical reactions

that take place on the surface of the wafer. Typical PECVD reactors are inductively coupled plasmas, but microwave discharges can also be used.
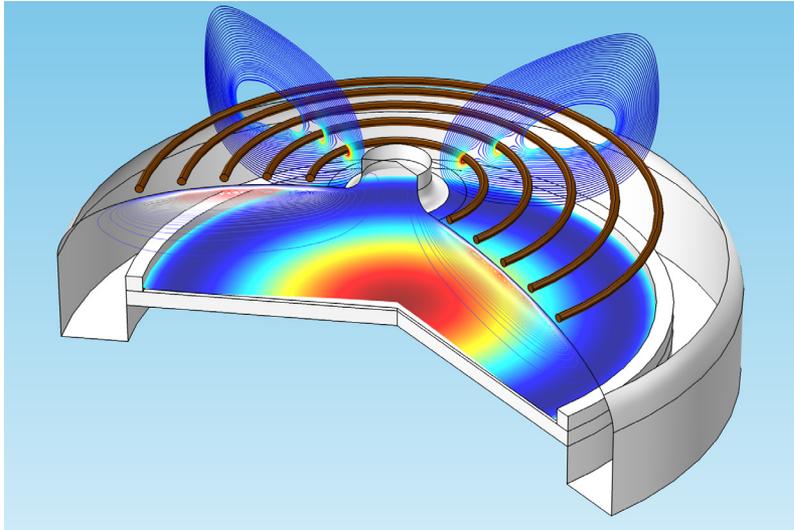

PECVD model of silicon deposition onto a wafer (surface) from a silane plasma. Silane is fed in from the shower head at the top and broken into radical species due to the presence of the electrons, which are sustained through induction heating.

DIELECTRIC BARRIER DISCHARGES

Dielectric barrier discharges (DBD) have many uses including light generation for plasma and LCD displays, ozone generation, and surface modification. The operating principle for a dielectric barrier discharge is as follows: there is a small gap filled with a gas in between two dielectric plates. The gap between the two dielectric plates is typically less than one millimeter. On one of the dielectric plates, a sinusoidal voltage is applied. The other plate is electrically grounded. As the voltage applied to the top plate increases, the electric field increases in the gap between the plates. Any free electrons in the gap will be accelerated and if the electric field is strong enough they may acquire enough energy to cause ionization. This can lead to a cascade effect where the number of electrons in the gap increases exponentially on a nanosecond time scale. Electrons created via electron impact ionization rush toward one of the dielectric plates, in the opposite direction to the electric field. An equal number of ions are also generated during electron impact ionization (electrons and ions must be created in equal pairs to preserve the overall charge balance). The ions rush toward the opposite dielectric plate in the same direction as the electric field. As a result, surface charge with opposite sign accumulates on both dielectric plates. This causes the electric field to become shielded from the gas filled gap. In fact, the electric field across the gap

cannot exceed the breakdown electric field, which is highly dependent on the gas and background pressure. The breakdown electric field is also a function of the surface properties of the dielectric material. Surface charge accumulation temporarily terminates the discharge until the field reverses direction and the process repeats in the opposing direction.

Surface: Mass fraction Ars (1)
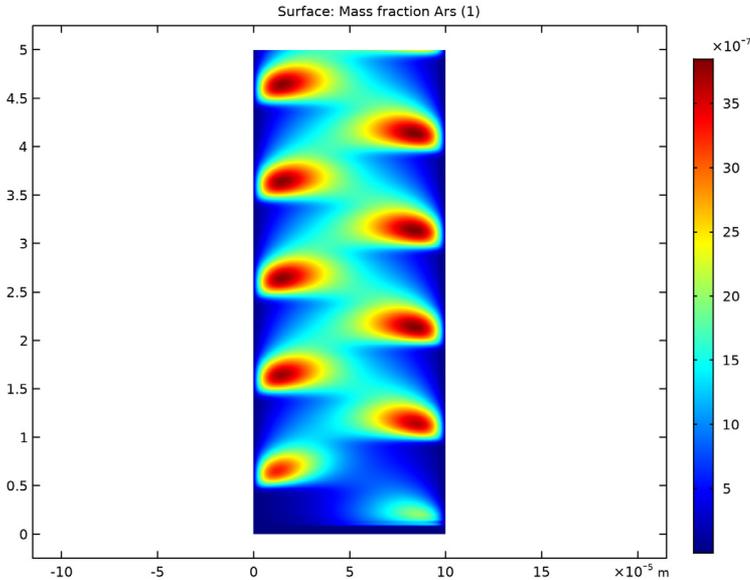
Dielectric Barrier Discharge: Plot of the mass fraction of electronically excited argon atoms in a dielectric barrier discharge. The x-axis represents space and the y-axis time. The applied frequency is 10 kHz.

Dielectric barrier discharges typically operate in the pressure range of 0.1–3 atm with an applied voltage of 1–100 kV and a frequency of kHz up to MHz. The dielectric barriers are usually made or quartz, glass, or a ceramic material. Electrode spacing is typically small, ranging from 100 μm up to several mm.

SPACE THRUSTERS AND MAGNETRON SPUTTERING

Magnetrons and space thrusters are essentially DC discharges aided by a static magnetic field. When the pressure is low enough (less than around 1 Pa), the magnetic field can trap the electrons so they are confined by the magnetic field lines, rather than escape to the walls. The trapping of the electrons results in more ionization collisions with the background gas and higher plasma densities than would normally be expected at such low pressures. Typical applied voltages are on the order of 500 V resulting in plasma currents on the order of amperes. The magnetic flux density is typically on the order of 0.01–0.15 T. Modeling

low-pressure magnetized DC discharges is very challenging, indeed most practical applications are beyond the current capabilities of the Plasma Module; see Limitations of the Plasma Module below.

EQUILIBRIUM DISCHARGES

Equilibrium discharges (sometimes called thermal plasmas) have a large range of industrial applications including: cutting, welding, spraying, waste destruction and surface treatment. Thermal plasmas are assumed to be under partial to complete local thermodynamic equilibrium (LTE) conditions. Under LTE, the plasma can be considered a conductive fluid mixture and therefore, be modeled using the magnetohydrodynamics (MHD) equations. The electron temperature is assumed to be equal to the temperature of the background gas. Equilibrium discharges are treated differently to the other examples above. The chemical composition of the plasma is not computed, only the gas temperature and electric fields. Sometimes the background velocity and pressure of the gas is also computed. These models allow the thermal loads on surfaces to be computed in a more efficient and stable way than using a non-equilibrium discharge model.

Plasma Modeling

There are three methods typically employed to model plasmas. All methods essentially involve solving an appropriate transport equation along with Maxwell's equations.

Kinetic	Fluid Approximation	Hybrid

- The Kinetic approach solves for the distribution function for the ions and electrons in a plasma by solving either the Boltzmann equation or an approximation, like the Fokker-Planck equation. The distribution function can also be computed using a Lagrangian approach, where ordinary differential equations are solved for the electron position and velocity, as is the case in particle-in-cell (PIC) codes. The advantage of this approach is that it allows for the electron energy distribution function to take an arbitrary shape in energy space and can also show effects that are not captured by fluid models. Drawbacks include difficulties associated with implementing arbitrary plasma chemistries and high computational cost.

- The Fluid approximation describes the plasma in terms of macroscopic quantities by assuming a specific form of the distribution function and taking velocity moments of the Boltzmann equation. This results in a set of coupled partial differential equations that can be solved using the finite element method. The Plasma Module uses the fluid approximation. Advantages of the fluid approximation are that it is efficient to solve the resulting equations and straightforward to define arbitrarily complex plasma chemistries. It is also easy to couple the electron dynamics to the electromagnetic fields, which are also computed using the finite element method.

- Hybrid methods treat some of the components of a plasma as a fluid and others kinetically. Usually, the electrons are treated kinetically by solving the Fokker-Planck equation or using a Monte Carlo method, and the ions and other radical species are computed using a fluid model. In this sense, hybrid methods offer a compromise between the fidelity of kinetic models and the speed and convenience of fluid models.

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 either by loading in sets of collision cross sections from a file or by adding reactions and species to the Model Builder.

Physics Guide

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.

Physics Interface List by Space Dimension and Preset Study Type

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
AC/DC				
Electrical Circuit		cir	Not space dependent	stationary; frequency domain; time dependent; small signal analysis, frequency domain
Electrostatics[1]		es	all dimensions	stationary; time dependent; stationary source sweep

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Fluid Flow				
Single-Phase Flow				
Laminar Flow[1]		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Plasma				
Boltzmann Equation, Two-Term Approximation		be	0D	mean energies; reduced electric fields
Plasma, Time Periodic		ptp	1D, 2D axisymmetric	time periodic; time periodic to time dependent
Plasma		plas	all dimensions	time dependent
Corona Discharge[4]		—	all dimensions	stationary
Inductively Coupled Plasma[2, 4]		—	3D, 2D, 2D axisymmetric.	frequency-transient
Microwave Plasma[3, 4]		—	3D, 2D, 2D axisymmetric	frequency-transient
Electrical Breakdown Detection		ebd	3D, 2D, 2D axisymmetric	time dependent
Equilibrium Discharges				
Equilibrium DC Discharge[4]		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Combined Inductive/ DC Discharge[2,4]		—	3D, 2D, 2D axisymmetric	frequency-transient
Equilibrium Inductively Coupled Plasma[2,4]		—	3D, 2D, 2D axisymmetric	frequency-transient
Species Transport				
Drift Diffusion		dd	all dimensions	time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Heavy Species Transport		hs	all dimensions	time dependent
Charge Transport		ct	all dimensions	stationary

[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.
[4] This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.

AC/DC INTERFACES

The AC/DC Branch chapter describes the two physics interfaces available with this module under the AC/DC branch of the Model Wizard. 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.

FLUID FLOW INTERFACES

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

BOLTZMANN EQUATION, TWO-TERM APPROXIMATION INTERFACE

The Boltzmann Equation, Two-Term Approximation interface computes the electron energy distribution function (EEDF) from a set of collision cross sections for some mean discharge conditions. The interface can be used as a preprocessing stage before solving a full space dependent model. The main purpose of this interface is to compute electron source coefficients and transport properties.

DRIFT DIFFUSION INTERFACE

The Drift Diffusion interface is used 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. This interface rarely needs to be used by itself as it makes up part of the application specific interfaces described later.

The Charge Transport interface computes the density of charge carriers in a background gas under the assumption that the transport is dominated by migration. This is typically only used as part of the Corona Discharge multiphysics interface (see below).

THE HEAVY SPECIES INTERFACE

The Heavy Species Transport interface ⠿ solves a mass balance equation 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, volumetric species, and surface species via the Model Builder. This interface rarely needs to be used by itself as it makes up part of the application specific interfaces described later.

ELECTRICAL BREAKDOWN DETECTION

The Electrical Breakdown Detection interfaces uses an approximate method to determine if electrical breakdown will occur in a given design by integrating Townsend growth coefficients along electric field lines.

Application Specific Interfaces

The Plasma Module provides four application specific multiphysics interfaces for modeling the most common types of discharge.

PLASMA

The Plasma interface ▦ can be used to model positive columns, glow discharges and corona 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.

PLASMA, TIME PERIODIC

The Plasma, Time Periodic interface ⚙ can be used to model capacitively coupled plasmas. Instead of solving the problem in the time domain, the periodic steady state solution is computed. This avoids having to solve for tens or hundreds of thousands of RF cycles, which is typically how long it takes before the plasma reaches the periodic steady state solution. This novel approach maintains all the non–linearity of the model while dramatically reducing computation time. The physics interface accomplishes this by attaching an extra dimension to the

underlying mathematical equations representing one RF cycle, and enforcing periodic boundary conditions in the aforementioned extra dimension.

Inductively Coupled Plasma

The Inductively Coupled Plasma interface ◉ can be used to model discharges sustained through induction currents. These discharges typically operate in the MHz frequency range. Inductively coupled plasmas (ICP) are important in plasma processing and plasma sources because the plasma density can be considerably higher than in capacitively coupled discharges. Inductively coupled plasmas are also attractive from the modeling perspective because they 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 when solving. As such, the quasi steady-state solution is reached in relatively few time steps.

Microwave Plasma

The Microwave Plasma interface ▦ can be used to model discharges which are sustained through heating of electrons due to electromagnetic waves. These discharges typically operate in the GHz frequency range. 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.

Corona Discharge

The Corona Discharge interface uses a simplified charge transport model coupled with electrostatics to provide an approximate method of computing the charge density and the electrostatic field in corona discharges.

Equilibrium Inductively Coupled Plasma

The Equilibrium Inductively Coupled Plasma ▦ multiphysics interface is used to study equilibrium discharges that are sustained by induction currents, for example in inductively coupled plasma torches. This multiphysics interface adds these single physics interfaces: Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling

of the equilibrium plasma by enthalpy transport, Joule heating and radiation loss. The multiphysics couplings also add the Lorentz forces to the hydrodynamics model.

Equilibrium DC Discharge

The Equilibrium DC Discharge 📊 multiphysics interface is used to study equilibrium discharges that are sustained by a static (or slowly varying) electric field where induction currents and fluid flow effects are negligible. This multiphysics interface adds an Electric Currents interface and a Heat Transfer in Fluids interface. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating and radiation loss.

Combined Inductive/DC Discharge

The Combined Inductive/DC Discharge 📊 multiphysics interface is used to study equilibrium discharges that are sustained by induction currents and static (slowly varying) electric field, for instance, in arc welding simulations. This multiphysics interface adds these single physics interfaces: Electric Currents, Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating and radiation loss. The multiphysics couplings also combine the induction and electrostatic currents as well as the Lorentz forces to the hydrodynamics model.

Limitations of the Plasma Module

The Plasma Module cannot currently model magnetrons and space thrusters due to the fact that the perpendicular versus cross field electron mobility and diffusivity can be on the order of 10^8. This poses severe numerical challenges and inevitably there is unphysical numerical diffusion across the magnetic field lines. As such, a truly self consistent model of a Hall thruster or magnetron is not currently possible, although it is still possible to gain valuable insight into the physics.

References

1. http://www-pub.iaea.org/mtcd/meetings/PDFplus/2010/cn180/cn180_papers/itr_p1-37.pdf.

2. G.J.M. Hagelaar, and L.C. Pitchford, "Solving the Boltzmann Equation to Obtain Electron Transport Coefficients and Rate Coefficients for Fluid Models," *Plasma Sources Sci. Technol*, vol. 14, pp. 722–733, 2005.

3. D.P. Lymberopolous and D.J. Economou, "Two-Dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell," *J. Res. Natl. Inst. Stand. Technol.*, vol. 100, pp. 473, 1995.

4. Annemie Bogaertsa, Erik Neytsa, Renaat Gijbelsa, Joost van der Mullen, "Gas discharge plasmas and their applications", *Spectrochimica Acta Part B*, vol. 57, pp. 609–658, 2002.

5. Michael A. Lieberman and Allan J. Lichtenberg, "Principles of Plasma Discharges and Materials Processing", Wiley (2005).

Argon Discharge in the GEC Reference Cell

The GEC cell was introduced by NIST in order to provide a standardized platform for experimental and modeling studies of discharges in different laboratories (Ref. 1). The plasma is sustained via inductive heating. The Reference Cell operates as an inductively-coupled plasma in this mode.

Inductively coupled discharges typically operate at low pressures (<10 Pa) and high charge density (>10^{17} m^{-3}). High density plasma sources are popular because low pressure ion bombardment can provide a greater degree of anisotropy on the surface of the wafer.
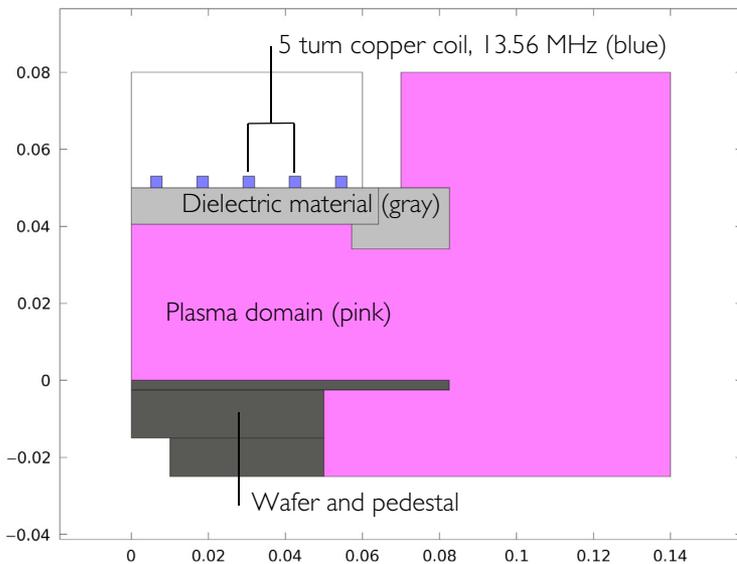
GEC ICP reactor geometry consisting of a 5-turn copper coil, plasma volume, dielectrics, and wafer with pedestal.

Because the physics occurring in an inductively coupled plasma is rather complex, it is always best to start a modeling project with a simple chemical mechanism. Argon is one of the simplest mechanisms to implement at low pressures. The

electronically excited states can be lumped into a single species, which results in a chemical mechanism consisting of only 3 species and 7 reactions:

LIST OF VOLUMETRIC PLASMA CHEMICAL REACTIONS CONSIDERED

REACTION	FORMULA	TYPE	$\Delta\varepsilon(eV)$
1	e+Ar=>e+Ar	Elastic	0
2	e+Ar=>e+Ars	Excitation	11.5
3	e+Ars=>e+Ar	Superelastic	-11.5
4	e+Ar=>2e+Ar+	Ionization	15.8
5	e+Ars=>2e+Ar+	Ionization	4.24
6	Ars+Ars=>e+Ar+Ar+	Penning ionization	-
7	Ars+Ar=>Ar+Ar	Metastable quenching	-

Stepwise ionization (reaction 5) can play an important role in sustaining low pressure argon discharges. Excited argon atoms are consumed via superelastic collisions with electrons, quenching with neutral argon atoms, and ionization or Penning ionization where two metastable argon atoms react to form a neutral argon atom, an argon ion and an electron. In addition to volumetric reactions, the following surface reactions are implemented:

LIST OF SURFACE REACTIONS CONSIDERED

REACTION	FORMULA	STICKING COEFFICIENT
1	Ars=>Ar	1
2	Ar+=>Ar	1

When a metastable argon atom makes contact with the wall, it will revert to the ground state argon atom with some probability (the sticking coefficient).

From an electrical point of view, the GEC reactor behaves as a transformer. A current is applied to the driving coil (the primary) and this induces a current in the plasma (the secondary). The plasma then induces an opposing current back in the coil, increasing its resistance. The current flowing in the plasma depends on the current applied to the coil and the reaction kinetics. The total plasma current can vary from no current (plasma not sustained) to the same current as the primary which corresponds to perfect coupling between the coil and the plasma. In this example, the coil is driven with a fixed power, 1500 W.

Model Wizard

The first step to build a model is to open COMSOL and then specify the type of analysis you want to do — in this case, a frequency-transient inductively coupled plasma analysis. The frequency-transient study type means that the high frequency electromagnetic field is computed in the frequency domain and all other variables are computed in the time domain.

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

1 Open COMSOL Multiphysics. In the New window, click the Model Wizard button .

2 In the Model Wizard window, click the 2D Axisymmetric button .

3 In the Select physics tree, select Plasma>Inductively Coupled Plasma .

4 Click the Add button.

5 Click the Study button .

6 In the tree, select Frequency-Transient .

7 Click Done .

Importing the Geometry

The next step is to create your geometry, which also can be imported from an external program. COMSOL Multiphysics supports a multitude of CAD programs and file formats. In this example, insert the prepared geometry sequence from a file in the COMSOL Multiphysics file format (.mph). The file contains the geometry of the GEC reference cell.

The location of the files used in this exercise varies based on your installation. For example, if the installation is on your hard drive, the file path might be similar to `C:\Program Files\COMSOL\COMSOL55\applications\`.

1 On the Geometry toolbar, click Insert Sequence .

2 Browse to the folder Plasma_Module\Inductively_Coupled_Plasmas under the COMSOL installation directory and double-click on the file `argon_gec_icp_geom.mph`.

3 Click the Import button. The geometry should appear in the Graphics window as shown below.
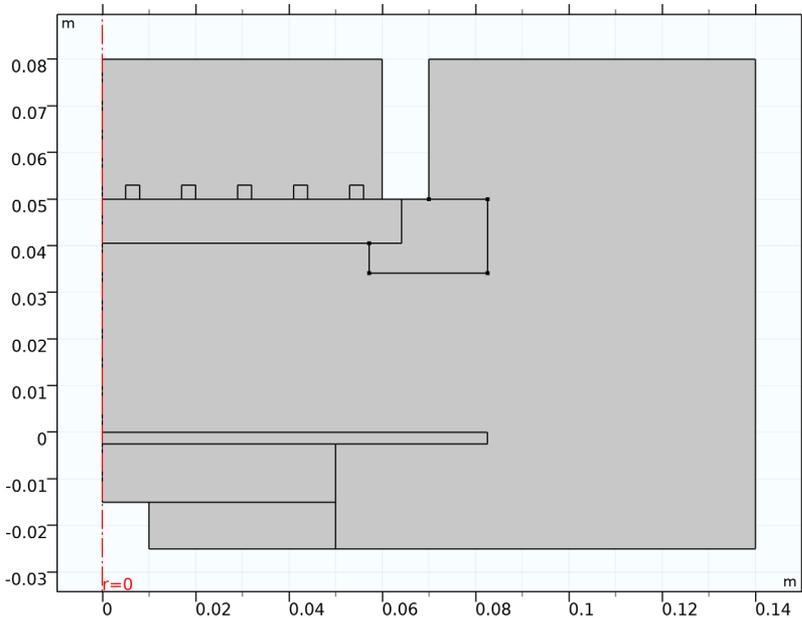
Definitions

1 On the Definitions toolbar, click Explicit 🐾.

2 In the Settings window, type `Walls` in the Label edit field.

3 Locate the Input Entities section.

4 From the Geometric entity level list, choose Boundary.

5 Go to the Home tab on the Model desktop toolbar, then choose Windows>Selection List.

6 Select Boundaries 6, 8, 35–38, 44, 45, and 51–56 only (by holding shown shift and clicking on the list), then click the Add to selection button ✚ at the top of the Selection List settings window. The selected boundaries in the graphics window will turn blue, indicating that the selection is confirmed.

7 Click back on the Model Builder tab.

8 On the Definitions toolbar, click Explicit 🐾.

9 In the Settings window, type `Coils` in the Label edit field.

10 Click on the Selection List tab and select Domains 6 and 8–11 only, then click the Add to selection button ✚ at the top of the Selection List settings window.

11 Click back on the Model Builder tab.

12 On the Definitions toolbar, click Explicit 🔖 .

13 In the Settings window, type `Coil Boundaries` in the Label edit field.

14 Click on the Selection List tab and select Domains 6 and 8–11 only, then click the Add to selection button ✚ at the top of the Selection List settings window.

15 Click back on the Model Builder tab. In the Explicit settings window, locate the Output Entities section.

16 From the Output entities list, choose Adjacent boundaries.

The settings for the selection should be as given below:
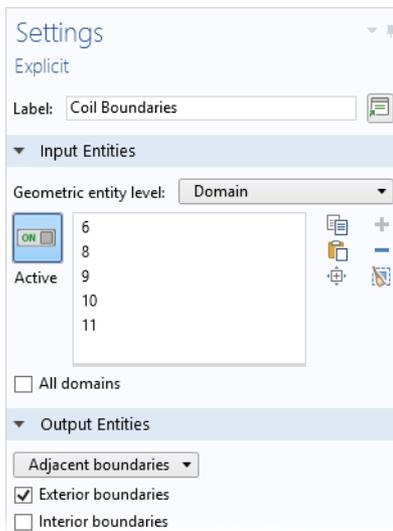
17 Go to the Model desktop toolbar.

18 On the Home toolbar, click Parameters Pᵢ and select Parameters 1 Pᵢ .

19 In the Parameters settings window, locate the Parameters section.

In the table, enter the following settings:

Name	Expression	Value	Description
Psp	1500[W]	1500 W	Power input
mueN	4E24[1/(m*V*s)]	4E24 1/(V·m·s)	Reduced electron mobility
T0	300[K]	300 K	Gas temperature
p0	0.02[torr]	2.6664 Pa	Gas pressure

Plasma and Magnetic Fields

1 In the Model Builder window, under Component 1 click on the Plasma node.

2 In the settings window, Locate the Plasma Properties section and select the Use reduced electron transport properties check box.

3 Click on the Selection List window. Select Domain 3 only.

4 In the Model Builder window, right-click Plasma and choose Cross Section Import.

5 In the Cross Section Import settings window, locate the Cross Section Import section.

6 Click the Browse button.

7 Browse to the module Application Library folder and double-click the file Ar_xsecs.txt.

Now you add two more regular reactions which describe how electronically excited argon atoms are consumed on the volumetric level. The rate coefficients for these reactions are taken from the literature.

1 In the Model Builder window, right-click Plasma and choose the domain setting Heavy Species Transport>Reaction .

2 In the Reaction settings window, locate the Reaction Formula section.

3 In the Formula edit field, type Ars+Ars=>e+Ar+Ar+. Click off the settings window.

4 Locate the Kinetics Expressions section. In the k^f edit field, type 3.734E8.

5 In the Model Builder window, right-click Plasma and choose the domain setting Heavy Species Transport>Reaction .

6 In the Reaction settings window, locate the Reaction Formula section.

7 In the Formula edit field, type `Ars+Ar=>Ar+Ar`. Click off the settings window.

8 Locate the Kinetics Expressions section. In the k^f edit field, type `1807`.

When solving any type of reacting flow problem there always needs to be one species which is selected to fulfill the mass constraint. This should be taken as the species with the largest mass fraction.

1 In the Model Builder window, under Component 1>Plasma click Species: Ar.

2 In the Species settings window, locate the Species Formula section.

3 Select the From mass constraint check box.

When solving a plasma problem the plasma must be initially charge neutral. COMSOL automatically computes the initial concentration of a selected ionic species such that the initial electroneutrality constraint is satisfied. Once the simulation begins to time step, the plasma need not be charge neutral. In fact, the separation of space charge between the ions and electrons close to the wall is a critical component in sustaining the discharge.

1 In the Model Builder window, under Component 1>Plasma click Species: Ar+.

2 In the Species settings window, locate the Species Formula section.

3 Select the Initial value from electroneutrality constraint check box.

Initial conditions for the electron number density and mean electron energy are critical for any plasma model. If the initial electron density is too low then the plasma may not be able to sustain itself and may self extinguish. If the initial electron density is too high then convergence problems may occur during initial time steps.

1 In the Model Builder window, under Component 1>Plasma click Initial Values 1.

2 In the Initial Values settings window, locate the Initial Values section.

3 In the $n_{e,0}$ edit field, type `1E15[1/m^3]`.

4 In the ε_0 edit field, type `5[V]`.

5 In the Model Builder window, under Component 1>Plasma click Plasma Model 1.

6 In the Plasma Model settings window, locate the Model Inputs section.

7 In the T edit field, type `T0`.

8 In the pA edit field, type `p0`.

9 Locate the Electron Density and Energy section. In the $\mu_e N_n$ edit field, type `mueN`.

Surface reactions must always be included in a plasma model since they describe how ionic, excited and radical species interact with the wall.

1 In the Model Builder window, under Component 1 right-click Plasma and choose the boundary condition Heavy Species Transport>Surface Reaction 🧪 .

2 In the Surface Reaction settings window, locate the Reaction Formula section.

3 In the Formula edit field, type `Ars=>Ar`.

4 Locate the Boundary Selection section. From the Selection list, choose Walls.

5 In the Model Builder window, right-click Plasma and choose the boundary condition Heavy Species Transport>Surface Reaction 🧪 .

6 In the Surface Reaction settings window, locate the Reaction Formula section.

7 In the Formula edit field, type `Ar+=>Ar`.

8 Locate the Boundary Selection section. From the Selection list, choose `Walls`.

Now add boundary conditions to describe how the electrons interact with the wall and specify that the walls are grounded.

1 In the Model Builder window, right-click Plasma and choose the boundary condition Drift Diffusion>Wall ⬭ .

2 In the Wall settings window, locate the General Wall Settings section.

3 In the r_e edit field, type `0.2`.

4 Locate the Boundary Selection section. From the Selection list, choose `Walls`.

5 In the Physics toolbar, click Boundaries and choose Ground ⬭ .

6 In the Ground settings window, locate the Boundary Selection section.

7 From the Selection list, choose `Walls`.

You need to compute the AC electric field both inside and outside the plasma. It is not necessary to compute the high frequency fields in the wafer or wafer pedestal, so start by modifying the selection for the Magnetic Fields interface.

1 In the Model Builder window, click Magnetic Fields.

2 Select Domains 3–6 and 8–12 only.

The Coil feature allows you to drive the system with a fixed total power. Some of this power will be dissipated in the coil, the rest will be coupled into the plasma. In this example 1500 W are applied to the system. This results in a plasma with a high number density. You also need to specify the gas temperature and pressure.

1 In the Model Builder window, right-click Magnetic Fields and choose the domain setting Coil ⬤ .

2 In the Coil settings window, locate the Domain Selection section.

3 From the Selection list, choose Coils.

4 Locate the Coil section. Select the Coil group check box.

In the Coil excitation, select Power and in the P$_{coil}$ edit field, type `Psp`.

Materials

Now assign material properties to the air, coil and dielectric domains.

1 In the Model Builder window, under Component 1 right-click Materials and choose Blank Material ⚏ .

2 In the Material settings window, locate the Geometric Entity Selection section.

3 From the Selection list, choose `Coils`.

4 Locate the Material Contents section. In the table, enter the following settings:

5 In the Model Builder window, under Component 1 right-click Materials and choose Blank Material ⚏ .

6 In the Material settings window, locate the Geometric Entity Selection section. Select Domain 5 only. In the table, enter the following settings:

7 In the Model Builder window, under Component 1 right-click Materials and choose Blank Material ⚏ .

8 In the Material settings window, locate the Geometric Entity Selection section. Select Domains 4 and 12 only. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permeability	mur_is...	1	1	Basic
Electrical conductivity	sigma...	0	S/m	Basic
Relative permittivity	epsilo...	4.2	1	Basic

Mesh

Meshing is a critical step in any plasma model. Boundary layer meshing on the reactor walls is nearly always necessary. This is needed to capture the separation of space charge between the electrons and ions close to the wall. You also add a fine mesh in the coil domains since the skin effect needs to be resolved.

1 In the Model Builder window, click Mesh 1 ⬛.

2 In the Mesh settings window, locate the Mesh Settings section.

3 From the Element size list, choose Finer.

4 Right-click Mesh 1 and choose More Operations>Edge ⬛.

5 Select Boundaries 6, 8, 44, 45, and 54 only.

6 Right-click Component 1>Mesh 1>Edge 1 and choose Size ⬛.

7 In the Size settings window, locate the Element Size section.

8 Click the Custom button.

9 Locate the Element Size Parameters section. Select the Maximum element size check box.

10 In the associated edit field, type `1E-3`.

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

12 In the Free Triangular settings window, locate the Domain Selection section.

13 From the Geometric entity level list, choose Domain.

14 Select Domain 3 only.

15 Right-click Component 1>Mesh 1>Free Triangular 1 and choose Size ▲.

16 In the Size settings window, locate the Element Size section.

17 From the Predefined list, choose Extra fine.

18 In the Model Builder window, right-click Mesh 1 and choose Boundary Layers ▧.

19 In the Boundary Layers settings window, locate the Domain Selection section.

20 From the Geometric entity level list, choose Domain.

21 Select Domain 3 only.

22 In the Model Builder window, under Component 1>Mesh 1>Boundary Layers 1 click Boundary Layer Properties ◭.

23 In the Boundary Layer Properties settings window, locate the Boundary Selection section.

24 From the Selection list, choose `Walls`.

25 Locate the Boundary Layer Properties section. In the Number of boundary layers edit field, type `5`.

26 In the Boundary layer stretching factor edit field, type `1.4`.

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

28 In the Mapped settings window, locate the Domain Selection section.

29 From the Geometric entity level list, choose Domain.

30 From the Selection list, choose `Coils`.

31 Right-click Component 1>Mesh 1>Mapped 1 and choose Distribution ▦.

32 In the Distribution settings window, locate the Boundary Selection section.

33 From the Selection list, choose `Coil Boundaries`.

34 In the Distribution settings window, locate the Distribution section.

35 From the Distribution type list, choose Predefined distribution type.

36 In the Number of elements edit field, type `25`.

37 In the Element ratio edit field, type `20`.

38 From the Growth formula list, choose Geometric sequence.

39 Select the Symmetric distribution check box.

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

**41** Right-click Mesh 1 and choose Build All ▦ .

Study

The model is now ready to be solved. You just need to enter the list of output times and the frequency for the induction currents.

1 In the Model Builder window, expand the Study 1 node, then click Step 1: Frequency-Transient 🗠.

2 In the Frequency-Transient settings window, locate the Study Settings section.

3 In the Times edit field, type 0 (the number zero followed by a space)

4 Click the Range button 🖿.

5 Go to the Range dialog box.

6 From the Entry method list, choose Number of values.

7 In the Start edit field, type -8.

8 In the Stop edit field, type -3.

9 In the Number of values field, type 21.

10 From the Function to apply to all values list, choose exp10. The text field should now contain 0 10^{range(-8,5/20,-3)}.

11 Click the Add button.

12 In the Frequency field, type 13.56E6.

13 In the Model Builder window, right-click Study 1 and choose Compute = .

Results

There are three default plots generated, one for the electron number density, one for the electron temperature and one for the electrostatic potential. After the model has solved, the default plot is of the electron density. The peak electron density occurs at the center of the reactor, underneath the RF coil. The electron

density in this case is high enough to cause some shielding of the azimuthal electric field.

Time=0.001 s   Surface: Electron density (1/m³)
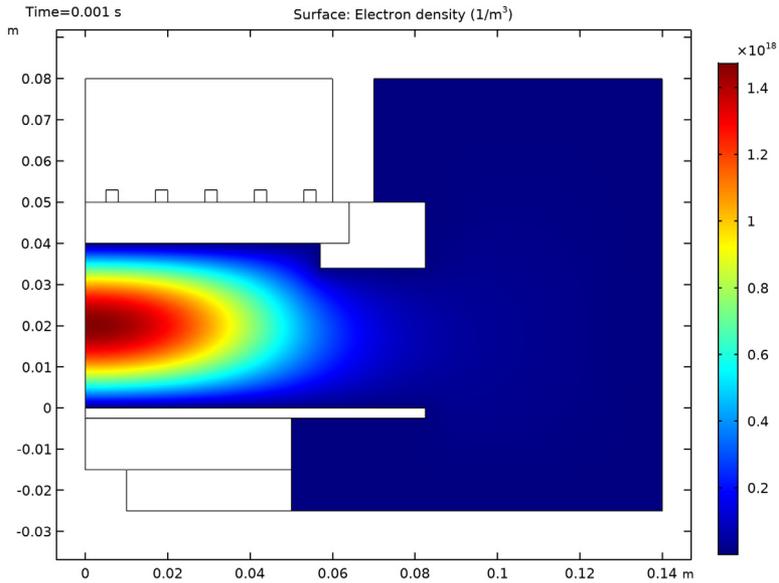
I To view the electron temperature, click on the Electron Temperature (plas) plot group ▮ .

The electron "temperature" is highest directly underneath the coil, which is where the bulk of the power deposition occurs.

Time=0.001 s   Surface: Electron temperature (V)
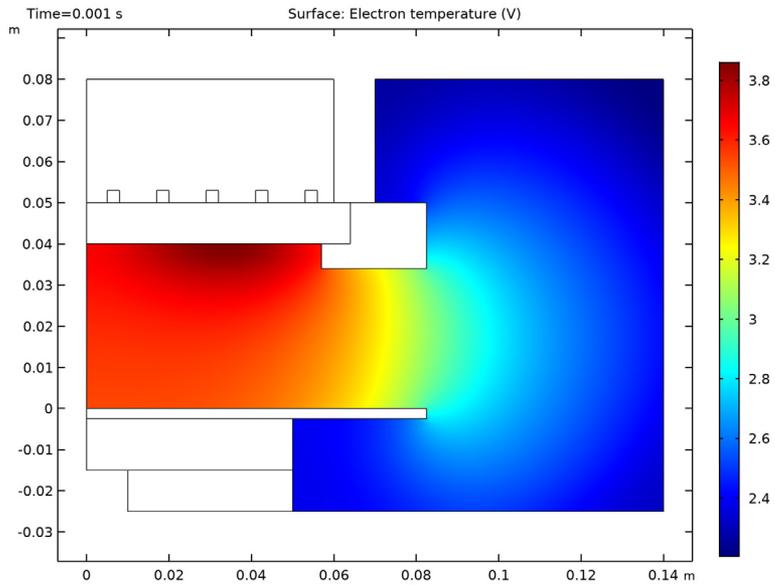
2 To view the electric potential, click on the Electric Potential (plas) plot
group ■ .

Time=0.001 s   Surface: Electric potential (V)
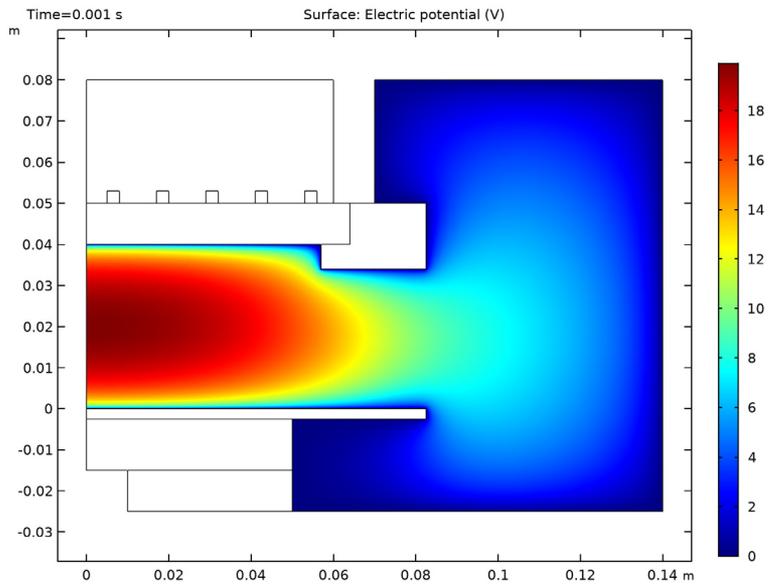
Now add a global plot for the coil resistance. This is defined as the real part of the total voltage drop over the coil divided by the current.

3 In the Model Builder window, right-click Results and choose 1D Plot Group 〰.

4 Right-click Results>1D Plot Group 6 and choose Global 〰.

5 In the Global settings window, locate the y-Axis Data section. Click Replace Expression ◣ ▾ . Select Magnetic Fields>Coil Parameters>Coil Resistance (mf.RCoil_1) from the list.

6 Click the x-Axis Log Scale button ▦ on the Graphics toolbar.

7 Click the Plot button ⊡ .

Global: Coil resistance (Ω)
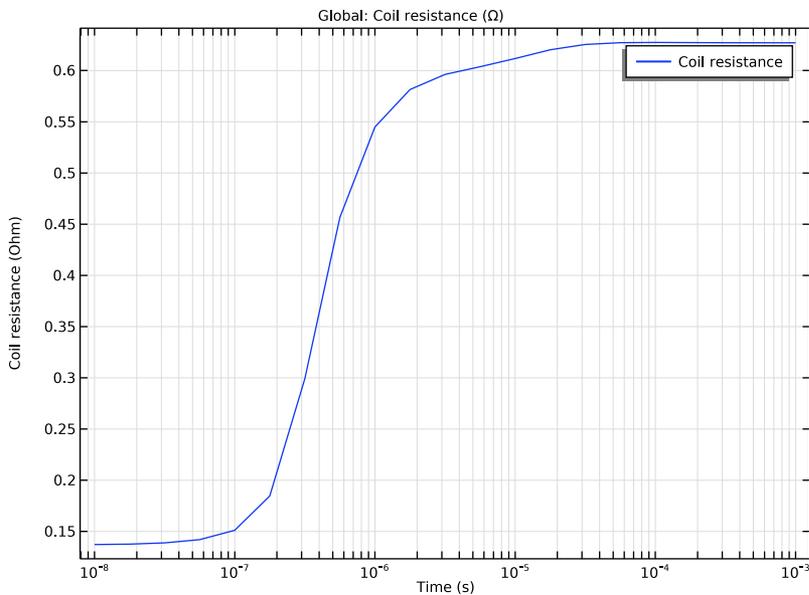
Now add a plot for the total power dissipated in the system. This is one half of the real part of the total voltage drop over the coil multiplied by the applied current.

8 In the Model Builder window, right-click Results and choose 1D Plot Group 〰.

9 Right-click Results>1D Plot Group 5 and choose Global.

10 In the Global settings window, locate the y-Axis Data section. Click Replace Expression ◣ ▾ . Select Magnetic Fields>Coil Parameters>Coil Power (mf.PCoil_1) from the list.

11 Click the x-Axis Log Scale button ▦ on the Graphics toolbar.

**12** Click the Plot button ⊡ .

Global: Coil power (W)
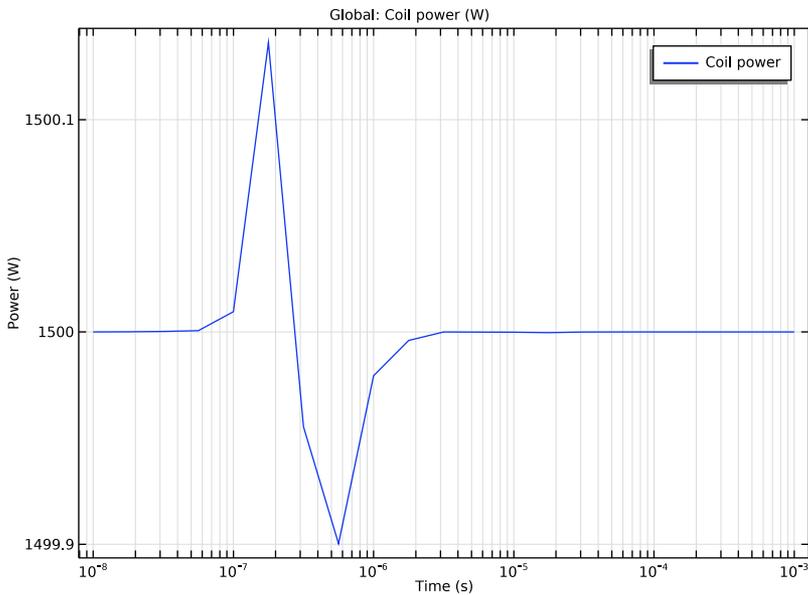
Now you add some additional two dimensional plots.

1 In the Model Builder window, right-click Results and choose 2D Plot Group ▪ .

2 Right-click 2D Plot Group 6 and choose Surface ▪ .

3 In the Surface settings window, click Replace Expression ▶▼ in the upper-right corner of the Expression section. From the menu, choose Plasma (Heavy Species Transport)>Number densities>Number density (plas.n_wAr_1p).

4 Click the Plot button ⊡ .

5 Click the Zoom Extents ⊕ button on the Graphics toolbar.

Time=0.001 s   Surface: Number density Ar+ (1/m³)
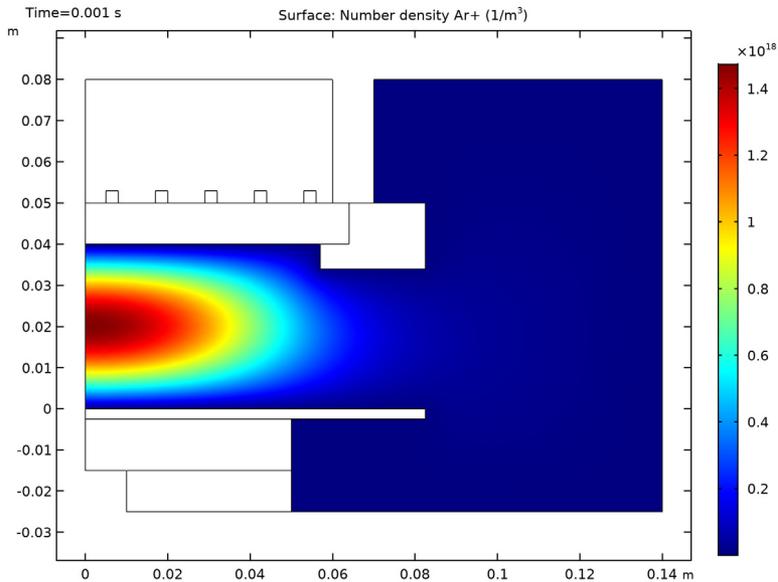
A quick way of creating additional plots is to use the Duplicate option. Now create a plot of the norm of the high frequency electric field.

6 In the Model Builder window, right-click 2D Plot Group 6 and choose Duplicate ⬚.

7 In the Model Builder window, expand the 2D Plot Group 7 node, then click Surface 1 ⬛.

8 In the Surface settings window, click Replace Expression ▸ ▾ in the upper-right corner of the Expression section. From the menu, choose Magnetic Fields>Electric>Electric field norm (mf.normE).

9 Click the Plot button ⬚.

10 Click the Zoom Extents button ⬚ on the Graphics toolbar.

Time=0.001 s   Surface: Electric field norm (V/m)
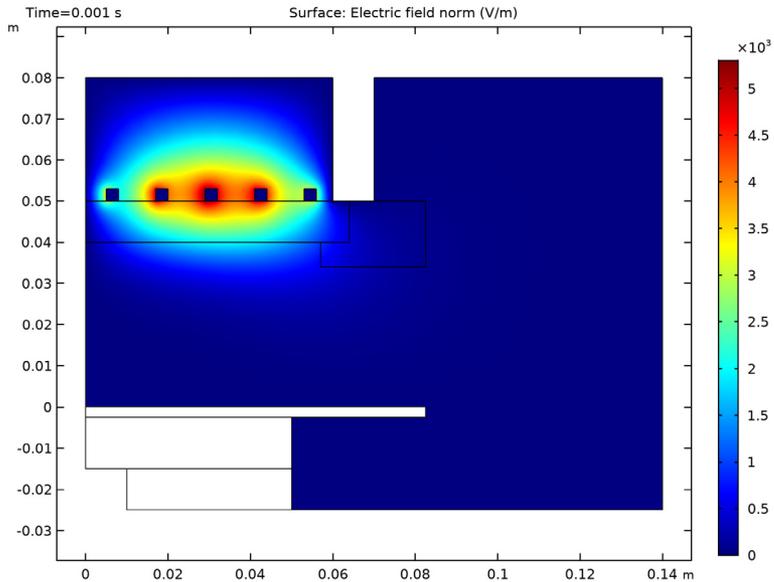
Observe that the electric field is slightly shielded by the plasma. This is due to the skin effect in the plasma. As the electron number density increases, the plasma tends to shield itself from the electric field. Now create a plot of the number density of electronically excited argon atoms.

11 In the Model Builder window, right-click 2D Plot Group 7 and choose Duplicate ⤵ .

12 In the Model Builder window, expand the 2D Plot Group 8 node, then click Surface 1 ▇ .

13 In the Surface settings window, click Replace Expression ⬐ ▾ in the upper-right corner of the Expression section. From the menu, choose Plasma (Heavy Species Transport)>Number densities>Number density (plas.n_wArs).

14 Click the Plot button ▣ .

15 Click the Zoom Extents button ⊕ on the Graphics toolbar.
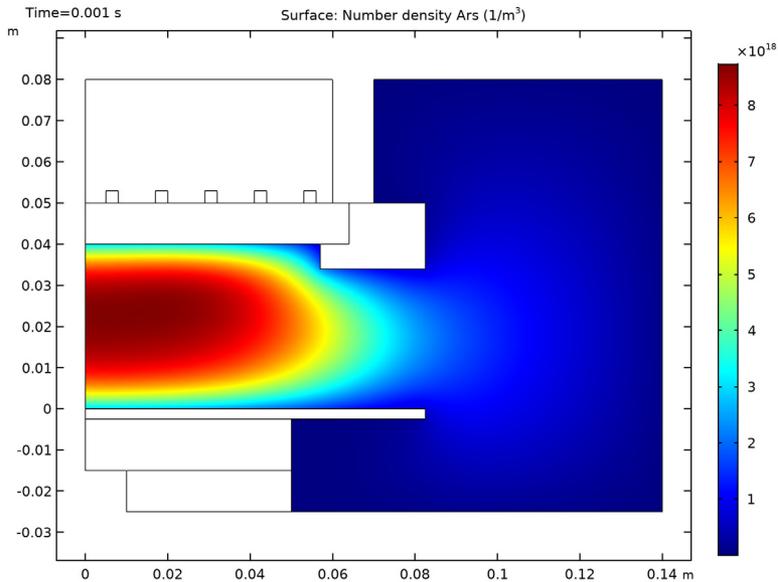
Finally, create a new data set only active on the plasma domain in order to make it easier to visualize the power deposition into the plasma.

1 In the Model Builder window, expand the Results>Data Sets node.

2 Right-click Solution 1 and choose Duplicate 🔁.

3 Right-click Results>Data Sets>Study 1/Solution 1 (2) and choose Selection.

4 In the Selection settings window, locate the Geometric Entity Selection section.

5 From the Geometric entity level list, choose Domain.

6 Select Domain 3 only.

7 Deactivate Propagate to lower dimensions.

8 In the Model Builder window, right-click Results and choose 2D Plot Group ■.

9 Right-click 2D Plot Group 9 and choose Surface ■.

10 In the Surface settings window, locate the Data section.

11 From the Data set list, choose Study 1/Solution 1(2).

12 Click Replace Expression ◀ ▼ in the upper-right corner of the Expression section. From the menu, choose Magnetic Fields>Heating and losses>Volumetric loss density (mf.Qrh).

13 Click the Plot button ▣.

14 Click the Zoom Extents button ⊕ on the Graphics toolbar.

Time=0.001 s   Surface: Volumetric loss density, electric (W/m³)
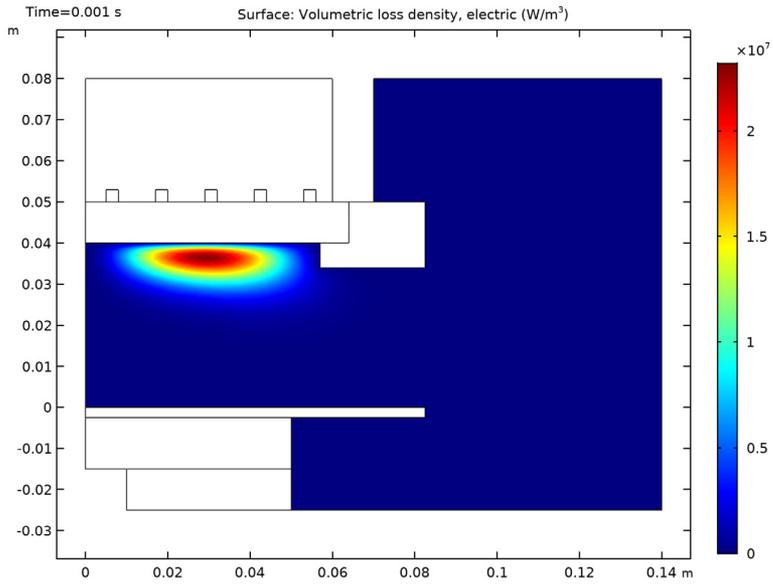
The effect of the shielding of the electric field due to the skin depth of the plasma is also apparent when plotting the power deposition.

Bibliography

1. D.P. Lymberopolous and D.J. Economou, "Two-Dimensional Self-Consistent Radio Frequency Plasma Simulations Relevant to the Gaseous Electronics Conference RF Reference Cell", *J. Res. Natl. Inst. Stand. Technol.*, vol. 100, pp. 473, 1995.