

GEC CCP Reactor, Argon Chemistry

Introduction

The NIST (National Institute of Standards and Technology) Gaseous Electronics Conference (GEC) Capacitively Coupled Plasma (CCP) reactor provides a standardized platform for studying capacitively coupled plasmas. Even the simplest plasma models are quite involved, so a 2D example helps in understanding the physics without excessive CPU time. The periodic steady state solution of an Argon discharge is computed and good agreement is obtained when comparing with measurements and simulations in the literature Ref. 1.

Model Definition

In this example, the GEC CCP reactor is simulated using the COMSOL Multiphysics Plasma Module. The simulations are for an Argon plasma sustained at a pressure of 100 mTorr by a periodic electric excitation of 13.56 MHz. The model is 2–dimensional and describes the space and time–periodic evolution of several macroscopic properties of the discharge. The reactor is electric asymmetric with a powered electrode of approximately 10 cm diameter and a gap between electrodes of 2.45 cm.

The mechanisms of power deposition into a CCP reactor is highly nonlinear and occurs at multiple different frequencies. Therefore, the electrostatic potential cannot be solved for in the frequency domain; the model must describe the periodic evolution of the charged particles to capture the nonlinear power absorption behavior.

ELECTRICAL EXCITATION

The driven electrode has a fixed power which computes the self DC bias. This corresponds to the following expression and set of constraints on the electric potential:

$$V_s = V_a \cos(2\pi f_p t + \alpha) + V_{dc,b}$$
(1)

$$0 = f_p \int_{\partial t \, \partial \Omega} (\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \mathbf{n} \cdot \mathbf{J}_d) dS dt$$
(2)

$$P_{rf} = f_p \int_{\partial t \, \partial \Omega} (V_s - V_{dc,b}) (\mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e + \mathbf{n} \cdot \mathbf{J}_d) dS dt .$$
(3)

The constraint in Equation 2 is used to compute the self DC bias, $V_{dc,b}$. The constraint in Equation 3 is used to compute the RF potential, V_a such that a fixed amount of power is deposited into the plasma.

PLASMA CHEMISTRY

Argon has 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 2 species and 3 reactions presented in Table 1. As in Ref. 1, the mass fraction of the metastable state is not computed. Electron impact cross-sections are obtained from Ref. 2.

REACTION	FORMULA	ТҮРЕ	$\Delta\epsilon(eV)$
I	e+Ar=>e+Ar	Elastic	0
2	e+Ar=>e+Ars	Excitation	11.5
4	e+Ar=>2e+Ar+	Ionization	15.8

TABLE I: TABLE OF COLLISIONS AND REACTIONS MODELED.

In addition to volumetric reactions, the following surface reaction is implemented:

TABLE 2: TABLE OF SURFACE REACTIONS.

REACTION	FORMULA	STICKING COEFFICIENT	SECONDARY EMISSION COEFFICIENT	MEAN ENERGY OF SECONDARY ELECTRONS (V)
1	Ar+=>Ar	0	0.07	5.8

The ion use his internal energy to extract one electron from the wall with a probability of 0.07 and a mean energy of 5.8 V. The sticking coefficient is zero meaning that losses to the wall are assumed to be due to migration only.

Results and Discussion

The results presented in this section are for 1 W of power absorbed by the plasma. The voltage and current at the power electrode are presented in Figure 1. The amplitude of the applied voltage excitation and the DC self bias are numerically found to be approximately 100 V and -78 V, respectively. A DC self bias is present because the reactor is electrically asymmetric. This voltage ensures that the period averaged conduction current through the powered electrode is zero. Note also that the current collected at the electrode is not sinusoidal, meaning that there is power absorbed at harmonics higher than the fundamental.

Figure 2 to Figure 6 present different period–averaged plasma quantities. Figure 2 shows that the plasma is more dense within the small gap and attains the maximum density off–axis, as in the simulations of Ref. 1 and the measurements from Overzet *et al* (taken from Ref. 1). As expected, the period averaged potential presents an off–axis maximum related

with the maximum of the plasma density, and a DC component at the powered electrode imposed by the calculated DC self–bias.

The ionization rate presented in Figure 6 also exhibits the off-axis behavior but the maximum does not coincide with the maximum electron density as reported in Ref. 1.

Due to the reactor electric asymmetry, the smaller electrode (the powered electrode in this simulation) has a larger sheath with more intense electric fields. The consequences are higher electron temperatures and power deposition near the powered electrode.

The period averaged electron temperature in the COMSOL Multiphysics Plasma Module is computed from

$$\langle T_e \rangle = \frac{2}{3} \langle n_{\varepsilon} / n_e \rangle \tag{4}$$

where the brackets represent the period averaged. To obtain electron temperatures similar to the ones in Ref. 1the average should be computed as

$$\langle T_e \rangle = \frac{2}{3} \frac{\langle n_e \rangle}{\langle n_e \rangle}.$$
 (5)

Figure 7 and Figure 8 shows profiles of the electron density along the axial and radial coordinate. These results are in good agreement with the data of figure 7 in Ref. 1 where simulations and measurements are compared.

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Figure 1: Plot of the V-I characteristics of the discharge. Note the significant self DC bias due to the asymmetry of the discharge.



Figure 2: Plot of the period averaged electron density.



Figure 3: Plot of the period averaged electron temperature.



Figure 4: Plot of the period averaged electric potential.



Figure 5: Plot of the period averaged power deposition to the electrons.



Figure 6: Plot of the period averaged ionization rate (note the units are non-SI in this plot, for easier comparison with Ref. 1).



Figure 7: Plot of the on-axis electron density. Here, x=0 corresponds to the driven electrode.



Figure 8: Plot of the radial electron density profile half way across the discharge gap.

References

1. J.P.Boeuf and L.C. Pitchford, "Two-dimensional model of a capacitively coupled rf discharge and comparisons with experiments in the Gaseous Electronics Conference reference reactor," *Physical Review E*, vol. 51, no .2, pp. 1376–1390, 1995.

2. Phelps database, www.lxcat.net, retrieved 2017.

Application Library path: Plasma_Module/Capacitively_Coupled_Plasmas/ argon_gec_ccp

Modeling Instructions

From the File menu, choose New.

```
NEW
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In the New window, click 🕙 Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, The Plasma, Time Periodic interface will be used to compute the periodic steady state solution for the GEC reference cell, using the Time Periodic study.
- 2 click and 2D Axisymmetric.
- 3 In the Select Physics tree, select Plasma>Plasma, Time Periodic (ptp).
- 4 Click Add.
- 5 Click 🔿 Study.
- 6 In the Select Study tree, select Preset Studies for Selected Physics Interfaces> Time Periodic.
- 7 Click 🗹 Done.

Add some parameters for the geometric dimensions, the frequency and the input power.

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
L	2.54[cm]	0.0254 m	Discharge gap
R1	5.38[cm]	0.0538 m	Inner radius
R2	10.16[cm]	0.1016 m	Outer radius
Hd	10.16[cm]	0.1016 m	Chamber height
dThick	3[mm]	0.003 m	Dielectric thickness
fO	13.56[MHz]	1.356E7 Hz	Frequency
P0	1[W]	I W	Power

GEOMETRY I

The geometry includes a point for the dielectric break, and three additional points to help create a mapped mesh later on. Since the **Plasma, Time Periodic** interface generates a

tremendous number of degrees of freedom, creating a geometry which can be efficiently meshed will help reduce computation time and memory requirements when solving.

Rectangle 1 (r1)

- I In the **Geometry** toolbar, click **Rectangle**.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type R1.
- 4 In the **Height** text field, type L.
- 5 Click 틤 Build Selected.

Rectangle 2 (r2)

- I In the **Geometry** toolbar, click **Rectangle**.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type R2-R1.
- 4 In the **Height** text field, type Hd.
- **5** Locate the **Position** section. In the **r** text field, type R1.
- 6 In the z text field, type -Hd/2+L/2.
- 7 Click 🟢 Build All Objects.
- **8** Click the $4 \rightarrow$ **Zoom Extents** button in the **Graphics** toolbar.

Point I (ptl)

- I In the **Geometry** toolbar, click **Point**.
- 2 In the Settings window for Point, locate the Point section.
- 3 In the r text field, type R1-dThick.
- 4 Click 🔚 Build Selected.

Point 2 (pt2)

- I Right-click Point I (ptI) and choose Duplicate.
- 2 In the Settings window for Point, locate the Point section.
- **3** In the **z** text field, type L.
- 4 Click 틤 Build Selected.

Point 3 (pt3)

- In the Model Builder window, under Component I (comp1)>Geometry I right-click
 Point I (pt1) and choose Duplicate.
- 2 In the Settings window for Point, locate the Point section.

- **3** In the **r** text field, type R2.
- 4 Click 틤 Build Selected.

Point 4 (pt4)

- I In the Model Builder window, under Component I (compl)>Geometry I right-click Point 2 (pt2) and choose Duplicate.
- 2 In the Settings window for Point, locate the Point section.
- **3** In the **r** text field, type R2.
- 4 Click 틤 Build Selected.

Line Segment 1 (Is1)

- I In the Geometry toolbar, click 🚧 More Primitives and choose Line Segment.
- 2 On the object pt2, select Point 1 only.

It might be easier to select the correct by using the **Selection List** window. To open this window, in the **Home** toolbar click **Windows** and choose **Selection List**. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)



- 3 In the Settings window for Line Segment, locate the Endpoint section.
- 4 Find the End vertex subsection. Click to select the 🔲 Activate Selection toggle button.
- 5 On the object **pt1**, select Point 1 only.

Add some mesh control edges to facilitate meshing without affecting the setup of the physics or postprocessing.

Mesh Control Edges 1 (mcel)

- I In the Geometry toolbar, click 🏠 Virtual Operations and choose Mesh Control Edges.
- 2 In the Settings window for Mesh Control Edges, locate the Input section.
- **3** Clear the **Include adjacent vertices** check box.
- **4** On the object **fin**, select Boundaries 4 and 9 only.
- 5 In the Geometry toolbar, click 📗 Build All.

Now that the geometry is defined, add some selections to facilitate the setup of the physics.

DEFINITIONS (COMPI)

Walls

- I In the Definitions toolbar, click 堶 Explicit.
- 2 In the Settings window for Explicit, locate the Input Entities section.
- **3** From the **Geometric entity level** list, choose **Boundary**.
- 4 Select the All boundaries check box.
- **5** Select Boundaries 2–12 only.
- 6 In the Label text field, type Walls.

Driven Electrode

- I In the **Definitions** toolbar, click 🐚 **Explicit**.
- 2 In the Settings window for Explicit, locate the Input Entities section.
- **3** From the Geometric entity level list, choose Boundary.
- **4** Select Boundary 2 only.
- 5 In the Label text field, type Driven Electrode.

Dielectric Contact

- I In the **Definitions** toolbar, click **here Explicit**.
- 2 In the Settings window for Explicit, locate the Input Entities section.
- **3** From the **Geometric entity level** list, choose **Boundary**.
- **4** Select Boundaries 4 and 6 only.
- 5 In the Label text field, type Dielectric Contact.

Grounded Walls

- I In the Definitions toolbar, click 🗞 Explicit.
- 2 In the Settings window for Explicit, locate the Input Entities section.
- 3 From the Geometric entity level list, choose Boundary.
- **4** Select Boundaries 3, 5, and 7–12 only.
- 5 In the Label text field, type Grounded Walls.

For the physics, we will solve for the heavy species only in the base geometry, and use 30 elements in the extra dimension which represents one RF period.

PLASMA, TIME PERIODIC (PTP)

- I In the Model Builder window, under Component I (compl) click Plasma, Time Periodic (ptp).
- **2** In the **Settings** window for **Plasma**, **Time Periodic**, locate the **Extra Dimension Settings** section.
- **3** In the $P_{\rm xd}$ text field, type 1/f0.
- 4 In the *N* text field, type 30.
- 5 From the Heavy species selection list, choose Base geometry.

Cross Section Import 1

- I In the Physics toolbar, click 🖗 Global and choose Cross Section Import.
- 2 In the Settings window for Cross Section Import, locate the Cross Section Import section.
- 3 Click 📂 Browse.
- **4** Browse to the model's Application Libraries folder and double-click the file Ar_xsecs_reduced.txt.

Species: Ar

- I In the Model Builder window, click Species: Ar.
- 2 In the Settings window for Species, locate the General Parameters section.
- 3 From the Preset species data list, choose Ar.
- 4 Locate the Species Formula section. Select the From mass constraint check box.

Species: Ars

Disable the metastable species, since this is not included in the reference paper.

I In the Model Builder window, right-click Species: Ars and choose Disable.

For the Argon ions, use the built in lookup table for the mobility, and the local field approximation for the ion temperature.

Species: Ar+

- I In the Model Builder window, click Species: Ar+.
- 2 In the Settings window for Species, locate the Species Formula section.
- **3** Select the **Initial value from electroneutrality constraint** check box.
- 4 Locate the General Parameters section. From the Preset species data list, choose Ar.
- 5 Click to collapse the Species Formula section. Click to expand the Mobility and Diffusivity Expressions section. From the Specification list, choose Specify mobility, compute diffusivity.
- 6 From the lon temperature list, choose Use local field approximation.
- 7 Click to expand the Mobility Specification section. From the Specify using list, choose Argon ion in argon.

Surface Reaction 1

- I In the Physics toolbar, click Boundaries and choose Surface Reaction.
- 2 In the Settings window for Surface Reaction, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.
- 4 Locate the Reaction Formula section. In the Formula text field, type Ar+=>Ar.
- **5** Locate the **Reaction Parameters** section. In the γ_f text field, type **0**.

Enter the temperature, pressure and electron mobility as defined in the reference.

Plasma Model I

- I In the Model Builder window, click Plasma Model I.
- 2 In the Settings window for Plasma Model, locate the Model Inputs section.
- **3** In the *T* text field, type 300[K].
- **4** In the *p*_A text field, type **0.1**[torr].
- **5** Locate the **Electron Density and Energy** section. From the **Electron transport properties** list, choose **Specify mobility only**.
- 6 In the μ_e text field, type $3E5[cm^2/(V*s)]/0.1$.

Wall I

- I In the **Physics** toolbar, click **Boundaries** and choose **Wall**.
- 2 In the Settings window for Wall, locate the Boundary Selection section.
- 3 From the Selection list, choose Walls.

4 Locate the General Wall Settings section. In the r_e text field, type 5/11.

It is much more stable to drive the electrode with a fixed power rather than a voltage. Activate computation of the DC self bias since that is included in the reference.

Metal Contact 1

- I In the Physics toolbar, click Boundaries and choose Metal Contact.
- 2 In the Settings window for Metal Contact, locate the Boundary Selection section.
- **3** From the Selection list, choose Driven Electrode.
- **4** Locate the **RF Source** section. In the $P_{\rm rf}$ text field, type P0.
- **5** In the f_p text field, type **f0**.
- 6 Locate the DC Source section. Select the Compute DC self-bias check box.

Dielectric Contact I

- I In the Physics toolbar, click Boundaries and choose Dielectric Contact.
- 2 In the Settings window for Dielectric Contact, locate the Boundary Selection section.
- 3 From the Selection list, choose Dielectric Contact.

Ground I

- I In the **Physics** toolbar, click **Boundaries** and choose **Ground**.
- 2 In the Settings window for Ground, locate the Boundary Selection section.
- 3 From the Selection list, choose Grounded Walls.

To minimize the number of degrees of freedom, take some time to create a mesh which is fine where the discharge is expected to show large gradients, and use a much coarser mesh elsewhere.

MESH I

Mapped I

- I In the Mesh toolbar, click I Mapped.
- 2 In the Settings window for Mapped, click to expand the Control Entities section.
- **3** Clear the **Smooth across removed control entities** check box.

Distribution I

- I Right-click Mapped I and choose Distribution.
- **2** Select Boundaries 4 and 5 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 In the Number of elements text field, type 4.

Distribution 2

- I In the Model Builder window, right-click Mapped I and choose Distribution.
- **2** Select Boundaries 2 and 3 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 20.
- 6 In the **Element ratio** text field, type 5.

Distribution 3

- I Right-click Mapped I and choose Distribution.
- **2** Select Boundaries 7 and 9 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the Number of elements text field, type 15.
- 6 In the Element ratio text field, type 10.
- 7 Select the Symmetric distribution check box.

Distribution 4

- I Right-click Mapped I and choose Distribution.
- **2** Select Boundaries 6, 8, 10, and 12 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 15.
- 6 In the Element ratio text field, type 8.
- 7 Select the Symmetric distribution check box.

Distribution 5

I Right-click Mapped I and choose Distribution.



2 Select Boundaries 1, 11, 13, and 14 only.

- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 25.
- 6 In the Element ratio text field, type 3.
- 7 Select the Symmetric distribution check box.
- 8 Click 📗 Build All.

The model will take about 20 minutes to solve, depending on hardware. Using **Results** while solving>, it is possible to visualize the evolution of the electron density at each nonlinear iteration. To do this, first get the initial value.

TIME PERIODIC STUDY

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, type Time Periodic Study in the Label text field.
- **3** In the Study toolbar, click $\underset{t=0}{\overset{U}{=}}$ Get Initial Value.

TIME PERIODIC STUDY

Solver Configurations

In the Model Builder window, expand the Time Periodic Study>Solver Configurations node.

Solution 1 (soll)

I In the Model Builder window, expand the Time Periodic Study>Solver Configurations> Solution I (soll) node.

Now choose that the electron density should be plotted while solving.

- 2 In the Model Builder window, expand the Time Periodic Study>Solver Configurations> Solution 1 (sol1)>Stationary Solver 1 node, then click Fully Coupled 1.
- **3** In the **Settings** window for **Fully Coupled**, click to expand the **Results While Solving** section.
- **4** Select the **Plot** check box.
- **5** In the **Study** toolbar, click **= Compute**.

Cycle through the default plots so that the results can be compared with the reference.

RESULTS

Current and Voltage, Metal Contact 1 (ptp)

Create a new plot for the period-averaged ionization rate.

Ionization Source, Period-Averaged

- I In the Home toolbar, click 🚛 Add Plot Group and choose 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, type Ionization Source, Period-Averaged in the Label text field.

Surface 1

- I Right-click Ionization Source, Period-Averaged and choose Surface.
- In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (comp1)>Plasma,
 Time Periodic>Reaction rates>ptp.Re_av Rate expression, period averaged 1/(m³·s).
- 3 Locate the Expression section. In the Unit field, type 1/(cm^3*s).
- 4 In the Ionization Source, Period-Averaged toolbar, click 💽 Plot.
- **5** Click the + **Zoom Extents** button in the **Graphics** toolbar.

Create some cut lines so the on-axis and radial period-averaged electron density can be visualized.

Cut Line 2D I

- I In the Model Builder window, expand the Results>Datasets node.
- 2 Right-click Results>Datasets and choose Cut Line 2D.
- 3 In the Settings window for Cut Line 2D, locate the Line Data section.

- 4 In row Point 2, set R to 0.
- 5 In row Point 2, set Z to 2[cm].
- 6 From the Snapping list, choose Snap to closest boundary.

On Axis Electron Density

- I In the **Results** toolbar, click \sim **ID** Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Dataset list, choose Cut Line 2D I.
- **4** In the **Label** text field, type On Axis Electron Density.

Line Graph I

- I Right-click **On Axis Electron Density** and choose **Line Graph**.
- 2 In the On Axis Electron Density toolbar, click 🗿 Plot.

Cut Line 2D 2

- I In the **Results** toolbar, click **Cut Line 2D**.
- 2 In the Settings window for Cut Line 2D, locate the Line Data section.
- 3 In row **Point I**, set **Z** to L/2.
- 4 In row Point 2, set R to R2.
- **5** In row **Point 2**, set **Z** to L/2.

Radial Electron Density

- I In the Results toolbar, click \sim ID Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Dataset list, choose Cut Line 2D 2.
- 4 In the Label text field, type Radial Electron Density.

Line Graph I

- I Right-click Radial Electron Density and choose Line Graph.
- 2 In the Radial Electron Density toolbar, click 💿 Plot.

Evaluate the RF and self DC bias potentials.

Global Evaluation 1

- I In the **Results** toolbar, click (8.5) **Global Evaluation**.
- In the Settings window for Global Evaluation, click Replace Expression in the upper-right corner of the Expressions section. From the menu, choose Component I (compl)>
 Plasma, Time Periodic>Metal Contact I>ptp.mctl.Va_per Voltage amplitude V.

- 3 Click Add Expression in the upper-right corner of the Expressions section. From the menu, choose Component I (compl)>Plasma, Time Periodic>Metal Contact l> ptp.mctl.Vdcb_per DC bias voltage V.
- 4 Click **= Evaluate**.

Finally, add a study to convert the solution into the time domain. This allows all variables to be plotted at instantaneous points in time, rather than period averaged quantities. This study runs in seconds.

ADD STUDY

- I In the Home toolbar, click $\sim\sim$ Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select

Preset Studies for Selected Physics Interfaces>Time Periodic to Time Dependent.

- 4 Click Add Study in the window toolbar.
- 5 In the Home toolbar, click ~ 2 Add Study to close the Add Study window.

STUDY 2

Step 1: Time Periodic to Time Dependent

- I In the Settings window for Time Periodic to Time Dependent, locate the Study Settings section.
- 2 Click Range.
- 3 In the Range dialog box, choose Number of values from the Entry method list.
- 4 In the **Stop** text field, type 1/f0.
- 5 In the Number of values text field, type 51.
- 6 Click Replace.
- **7** In the Settings window for Time Periodic to Time Dependent, click to expand the Values of Dependent Variables section.
- 8 Find the Values of variables not solved for subsection. From the Settings list, choose User controlled.
- 9 From the Method list, choose Solution.
- 10 From the Study list, choose Time Periodic Study, Time Periodic.
- II In the Model Builder window, click Study 2.
- 12 In the Settings window for Study, type Time Periodic to Time Dependent in the Label text field.

I3 In the **Home** toolbar, click **= Compute**.

Create an animation of the electric potential.

RESULTS

Electric Potential (ptp)

In the Model Builder window, under Results click Electric Potential (ptp).

Animation I

In the Electric Potential (ptp) toolbar, click **IIII** Animation and choose Player.

Electron Density, Period Averaged (ptp)

Set a thumbnail image for the plot of the period-averaged electron density.

ROOT

- I In the Model Builder window, click the root node.
- 2 In the root node's Settings window, locate the Presentation section.
- 3 Find the Thumbnail subsection. Click Set from Graphics Window.