

# Simulation for a Plasma Discharge Model in Microwave Transmitter-Receiver Waveguide by COMSOL Multi Physics Software

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## ABSTRACT

Rapid plasma formation and evolution during microwave gas discharge device produce a macroscopic plasma shield to the microwave transmission, which can severely limit the performance of the device. In this paper, the electromagnetic (TE)- plasma interaction and the chlorine Discharge Global modelled in a standard rectangular waveguide WR 284 (72.14 mm× 32.04 mm) by COMSOL multi physics which provide to be a very good compromise between flexibility and work efficiency.

**Keyword:** Plasma discharge, Rectangular waveguide, S-Parameter, COMSOL Multiphysics, Microwave

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## INTRODUCTION

In the recent years, plasma discharge technology has been extensively developed. When microwave propagates in a waveguide with two symmetric metal pins, the discharge phenomenon can be found [1]. Many scientists focus on investigating EM propagation in the waveguide theoretically or experimentally [2, 3]. Discharge can be induced near geometrical discontinuities in a microwave device during the transmission of electromagnetic (EM) fields with a high-power density through a typical gas.

If the field intensity of the incident microwave exceeds a certain critical value, the electrons bound in the neutral atoms and molecules in gas can acquire enough

energy and become free electrons, accelerated by the high-intensity EM field [4].

The motion of the electrons produces an impact on other gas particles and releases free electrons into the device. These electrons are further accelerated by the EM fields and also impact other gas particles.

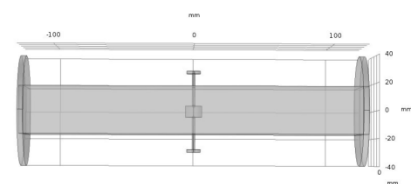


Fig.1: simulation model

Meanwhile, they also generate secondary EM fields that either enhance or weaken the incident fields. With sufficiently high-power density, an exponential increase of the number of electrons can occur, which is known as breakdown. When breakdown happens, the transmission capability of a microwave device can be severally limited[4]. In order to study the related EM-plasma interaction, physical models have to be constructed and simulated. In general, the EM fields and waves are governed by Maxwell's equations, while the plasma physics can be described by the Boltzmann's equation [5].

This paper is organized as follows: Section 2 describes the physical model in more details, and Electromagnetic field model is in section 3. In section 4 we discuss the plasma model, section 5 we present the simulation result, and conclusions are presented in section 6.

## PHYSICAL MODEL

We designed a simulation model of the standard waveguide WR284 (72.14mm ×32.04mm), and the radius of the cylindrical-shaped pins was 1mm with hemispherical ends, as shown in Fig. 1.

The core of the physical model is composed of plasma discharge by EM microwave. This set up requires a specific geometry, the definition of the rectangular port for receiving microwave, defining the boundary conditions, the chemical reactions rate and the transport coefficients. We use three studies in our component and couple them by multi physics option. These studies are Electromagnetic waves, Frequency Domain (emw), Electrostatic (es) and plasma (plas)[6].

## ELECTROMAGNETIC FIELD MODEL

The electromagnetic field model solves the wave equation in the time-harmonic approximation[6]

$$\nabla \times [\mu^{-1}(\nabla \times E)] - k_0^2 \left( \hat{\epsilon} - i \frac{\sigma}{\omega \epsilon_0} \right) \hat{\sigma} E = 0 \quad (1)$$

The internal volume of the reactor is then perceived as a dielectric with spatially inhomogeneous complex dielectric function[6, 7]

$$\epsilon = \epsilon_0 - \frac{\epsilon_0 \omega p_e^2}{v_{en}^2 + \omega^2} - i \frac{\epsilon_0 \omega p_e^2 v_{en}}{(v_{en}^2 + \omega^2)} \quad (2)$$

In the Equ (2),  $\epsilon_0$  denote vacuum permittivity,  $\omega = 2\pi f$  is the angular frequency of the EM radiation,  $\omega_{pe}$  is the plasma frequency and  $v_{en}$  is the total electron-neutral collision frequency.

The most important input for the EM field model is the electron  $n_e$  and temperature. This model shows a standard rectangular plasma waveguide how to work for microwaves.

We applied the transversal electric (TE) waves. These types of waves, don't have electric field component in direction of propagation so that TE<sub>01</sub> is the single propagation mode. The waveguide walls are typically plated with a very good conductor. In this model the walls are considered to be made of a perfect conductor, so  $n \times E = 0$  is on the boundaries. The rectangular port is excited by a transverse (TE) wave.

With the stipulated excitation at the rectangular port, the Equ (1) is solved for the electric field vector E inside the waveguide. Where  $\mu$  denotes the permeability,  $j$  the imaginary unit,  $\sigma$  the conductivity,  $\omega$  the angular frequency,  $\epsilon$  the permittivity, and  $\epsilon_0$  the permittivity of free space. Naming the rectangular port as port1 and port2, the S-parameters describing the reflection and transmission of the wave are defined as follows [6].

$$S_{11} = \frac{\int_{port1} ((E_c - E_1) \cdot E_1^*) dA_1}{\int_{port1} (E_1 \cdot E_1^*) dA_1} \quad (3)$$

$$S_{21} = \frac{\int_{port2} (E_c \cdot E_2^*) dA_2}{\int_{port2} (E_2 \cdot E_2^*) dA_2} \quad (4)$$

Here  $E_c$  is the calculated total field.  $E_1$  is analytical mode for the port excitation, and  $E_2$  is the eigen mode calculated from the Boundary mode analysis and normalized by outgoing power flow.

## PLASMA MODEL

The plasma model is very important in this paper. We solved the continuity equations for ions, electrons and excited species in the following form[7].

$$\frac{\partial n_j}{\partial t} + \pi \cdot \Gamma_j + (U \cdot \pi)_{n_j} = R_j \quad (5)$$

In this paper we determined the electron density absorbed power between 25 and 600w and work pressures between 1 and 100 m Torr.

To explore such a large parametric region, it is used a global (volume- averaged) model since it can run simulations in a fraction of time in space dependent model while retaining the tendencies of volume-averaged physical quantities. For heavy species the following equation is solved for the mass fraction.

$$V\rho \frac{d}{dt}(\omega_k) = m_f m_{f,k} - m_0 \omega_k + VR_k + \sum h_l A_l R_{surf,k,l} M_k - \omega_k \sum h_e A_l M_{f,l} \quad (6)$$

When  $m_f$  is the mass density (SI unit:  $kg/m^3$ ),  $\omega_k$  is the mass fraction,  $\omega_{f,k}$  is the mass fraction in the feed,  $M_f$  and  $m_0$  are the mass flow rates of the total feed and outlet, and  $R_k$  is the rate expression (SI unit:  $kg/m^3.s$ ). The forth the term in the right hand side equation, shows accounts for surface losses and creation, where  $A_l$  is the surface  $an_{em}$ ,  $h_l$  is a dimension less correction term,  $V$  is the reactor volume,  $M_k$  is the species molare mass (SI unit:  $kg/mol$ ) and  $R_{surf,k,l}$  is the surface rate expression (SI unit:  $mol/(m^2.s)$ ) at a surface  $l$  [7]

By taking into account possible variations of the system total mass or pressure the mass continuity equation can also be solved

$$V \frac{d\rho}{dt} = m_f - m_0 + \sum h_l A_l M_{f,l} \quad (7)$$

The electron number density is obtained from electron neutrality:

$$n_e = \sum_{k=1}^N Z_k n_k \quad (8)$$

And electron energy density  $n_e$  (unit:  $V/m^3$ ) is computed from

$$V \frac{dn_\epsilon}{dt} = VR_\epsilon + \frac{P_{abs}}{e} + \sum_l \sum_{ions} h_l A_l R_{surf,k,l} N_a (\epsilon_e + \epsilon_i) \quad (9)$$

When  $R_\epsilon$  is the electron energy loss due to inelastic and elastic collisions,  $P_{abs}$  is the power absorbed by the electron (SI unit:  $w$ ), and  $e$  is the elemental charge [7]. The summation is over positive ions,  $\epsilon_e$  is the mean kinetic energy lost per electron lost,  $\epsilon_i$  is the mean kinetic energy lost per ion lost, and  $N_a$  is the Avogadro's number. It is used the plasma chemistry suggested in [7] and presented in Table 1 which consists of 10 species and 44 reactions.

**Table 1:** Table collisions and reactions modelled [7]

REACTION	FORMULA	TYPE	$\Delta\epsilon(Ev)$
1	$e+Cl_2 \Rightarrow e+Cl_2$	Momentum	0
2	$e+Cl \Rightarrow e+Cl$	Momentum	0
3	$e+Cl_2 \Rightarrow Cl+Cl+e$	Dissociation	4
4	$e+Cl_2 \Rightarrow 2e+Cl_2+$	Ionization	11.5
5	$e+Cl_2 \Rightarrow 2e+Cl+Cl+$	Ionization	14.25
6	$e+Cl_2 \Rightarrow 3e+2Cl+$	Ionization	28.5
7	$e+Cl_2 \Rightarrow Cl+Cl-$	Attachment	0
8	$e+Cl_2v1 \Rightarrow Cl+Cl-$	Attachment	0
9	$e+Cl_2v2 \Rightarrow Cl+Cl-$	Attachment	0
10	$e+Cl_2v3 \Rightarrow Cl+Cl-$	Attachment	0
11	$e+Cl_2 \Rightarrow Cl++Cl+e$	Ionization/ Attachment	14.25
12	$e+Cl_2 \Rightarrow e+Cl_2v1^*$	Excitation	0.07
13	$e+Cl_2 \Rightarrow e+Cl_2v2^*$	Excitation	0.14
14	$e+Cl_2 \Rightarrow e+Cl_2v3^*$	Excitation	0.21
15	$e+Cl_2v1 \Rightarrow e+Cl_2v2^*$	Excitation	0.07
16	$e+Cl_2v2 \Rightarrow e+Cl_2v3^*$	Excitation	0.07
17	$e+Cl_2v1 \Rightarrow e+Cl_2v3^*$	Excitation	0.14
18	$e+Cl_2 \Rightarrow 2Cl$	Excitation	0
19	$e+Cl \Rightarrow e+Cl_{12}^*$	Excitation	1.35
20	$e+Cl \Rightarrow +Cl_{52}^*$	Excitation	10.17
21	$e+Cl \Rightarrow Cl++2e$	Ionization	14.25
22	$e+Cl_{12} \Rightarrow Cl++2e$	Ionization	10.18
23	$e+Cl_{52} \Rightarrow Cl++2e$	Ionization	4.08
24	$e+Cl- \Rightarrow Cl+2e$	Ionization	2.36
25	$e+Cl- \Rightarrow Cl++3e$	Ionization	16.61
26	$Cl_{52} \Rightarrow Cl$	Radiation decay	0

27	$\text{Cl}_2 + \text{Cl}^- \Rightarrow 3\text{Cl}$	Ion-ion recombination	0
28	$\text{Cl}_2 + \text{Cl}^- \Rightarrow \text{Cl} + \text{Cl}_2$	Ion-ion recombination	0
29	$\text{Cl} + \text{Cl}^- \Rightarrow 2\text{Cl}$	Ion-ion recombination	0
30	$\text{Cl}_2 + \text{Cl}^+ \Rightarrow \text{Cl} + \text{Cl}_2$	Charge exchange	0
31	$\text{Cl}_2\text{v}1 + \text{Cl}^+ \Rightarrow \text{Cl} + \text{Cl}_2^+$	Charge exchange	0
32	$\text{Cl}_2\text{v}2 + \text{Cl}^+ \Rightarrow \text{Cl} + \text{Cl}_2^+$	Charge exchange	0
33	$\text{Cl}_2\text{v}3 + \text{Cl}^+ \Rightarrow \text{Cl} + \text{Cl}_2^+$	Charge exchange	0
34	$2\text{Cl} + \text{Cl}_2 \Rightarrow 2\text{Cl}_2$	Association	0
35	$2\text{Cl} + \text{Cl} \Rightarrow \text{Cl}_2 + \text{Cl}$	Association	0
36	$\text{Cl} + \text{Cl}_2\text{v}3 \Rightarrow \text{Cl} + \text{Cl}_2\text{v}2$	Deexcitation	0
37	$\text{Cl} + \text{Cl}_2\text{v}2 \Rightarrow \text{Cl} + \text{Cl}_2\text{v}1$	Deexcitation	0

\*The reaction set includes the inverse reaction with the rate coefficient obtained by detailed balance.

The model also includes the surface reactions presented in Table 2.

**Table 2:** Table of surface reactions [7]

REACTION	FORMULA	STICKING COEFFICIENT
1	$\text{Cl}_2^+ \Rightarrow \text{Cl}_2$	1
2	$\text{Cl}^+ \Rightarrow \text{Cl}$	1
3	$\text{Cl}_2\text{v}1 \Rightarrow \text{Cl}_2$	1
4	$\text{Cl}_2\text{v}2 \Rightarrow \text{Cl}_2$	1
5	$\text{Cl}_2\text{v}3 \Rightarrow \text{Cl}_2$	1
6	$\text{Cl}_{12} \Rightarrow \text{Cl}$	1
7	$\text{Cl}_{52} \Rightarrow \text{Cl}$	1
8	$\text{Cl} \Rightarrow 0.5\text{Cl}_2$	Ref.1

The rate at which positive ions are lost to the wall is computed from the Bohm velocity and the density that an ion has near the surface. The ion density at the surface is estimated.

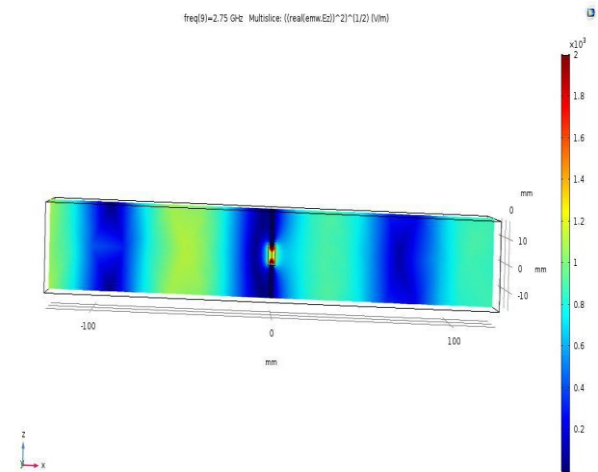
## SIMULATION RESULT

To answer these investigations, plasma discharge chlorine has been studied. In this paper, we simulated the chlorine discharge global by enhancing the electric field in a waveguide [7]. As shown in Fig.1, two metal pins were put on simulation model which carried out at 2-4 GHz microwave, and [25-600] w power. The advantages of this simulation set up are the electric strength near the pinpoint can be conveniently changed by adjusting the distance between the two pins shown in Fig.2, and it can be done under different circumstances such as different gas pressure and temperatures. We have used chlorine-global-model of plasma modules in COMSOL to investigate the interaction between EM microwaves and plasma discharge in a typical standard waveguide WR 284.

The effect of the pins on propagation of the microwaves is that the microwaves can reflect less if the discharge does not happen [8].

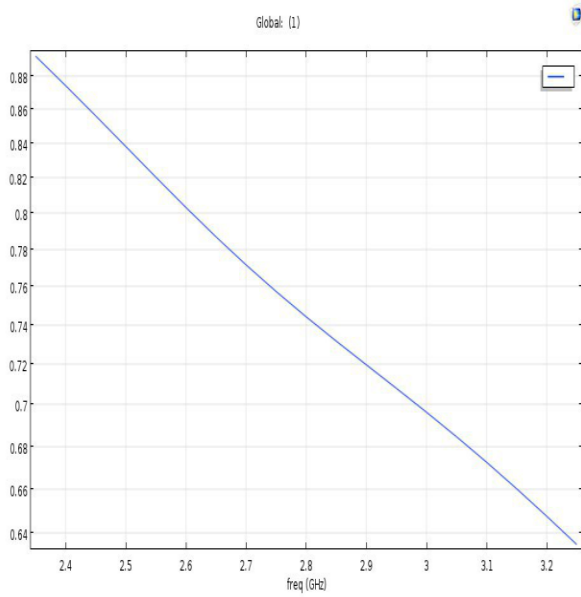
However, when the discharge happens the plasma will fill the gap and will increase the reflection greatly. At the same time, the microwave will be absorbed by the

plasma, and the result is decreasing the transmitted microwaves power [9].

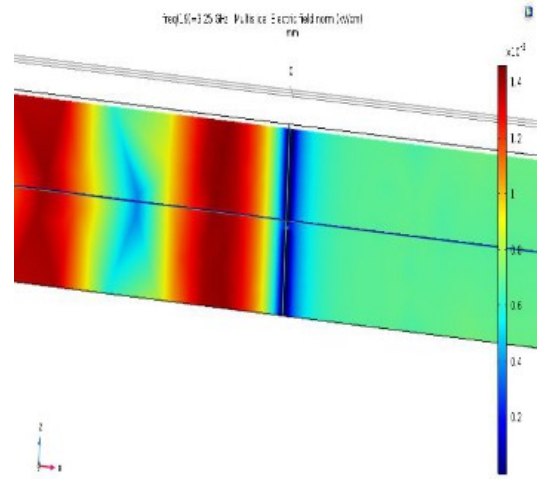


**Fig.2.:** (Colour online) Electric field in the waveguide

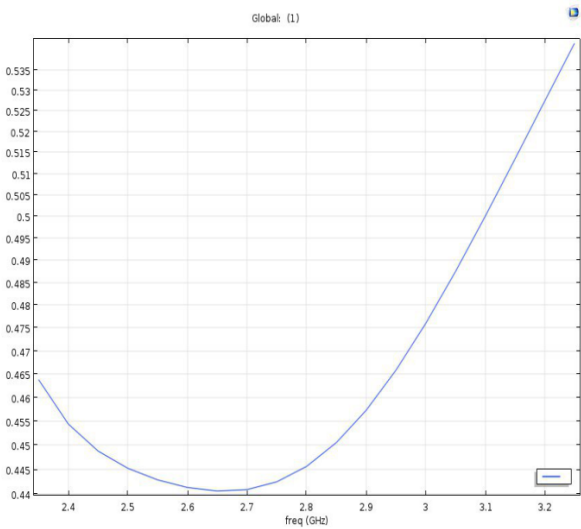
As shown in Fig.2 apparently, the electric field at the top of the metal pin is greatly strengthened. In addition, microwave reflectance, as long as the transmission power is obviously changed along with distance D (D represents the distance between the two pins), changed between the two pins [10].



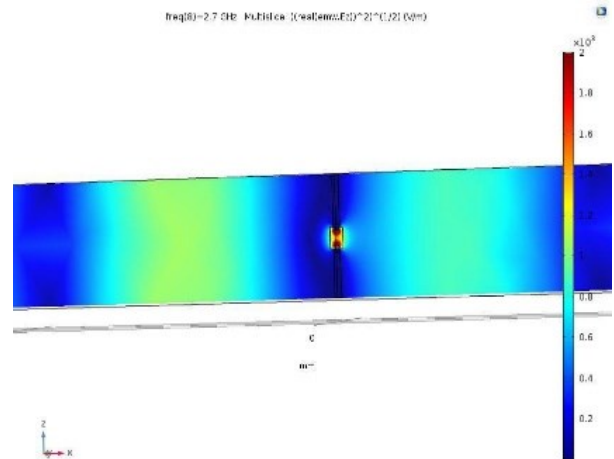
**Fig.3:** Reflectance  $S_{11}$  versus microwave frequency for  $D = 0$  mm and  $P = 0.01$  Torr



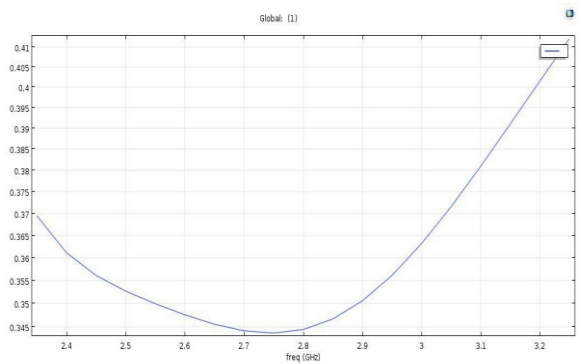
**Fig.4:** Electric field profile for  $D = 0$  mm at  $f = 2.8$ GHz



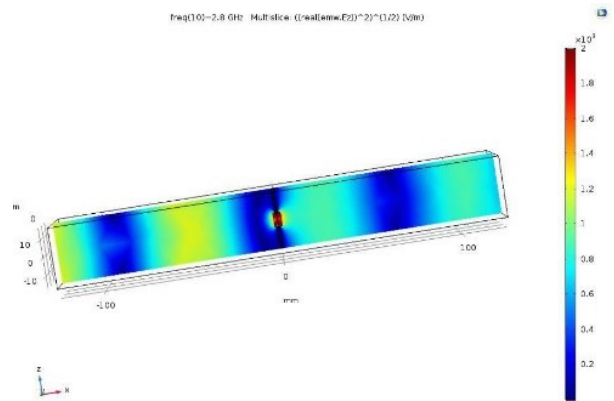
**Fig.5:** Reflectance  $S_{11}$  versus microwave frequency for  $D = 4$  mm and  $P = 0.01$  Torr



**Fig.6:** Electric field profile for  $D = 4$  mm at  $f = 2.8$ GHz



**Fig.7:** Reflectance  $S_{11}$  versus microwave frequency for  $D = 6$  mm and  $P = 0.01$  Torr



**Fig.8:** Electric field profile for  $D = 6$  mm at  $f = 2.8$ GHz

We employ a microwave at S-band of about 2.8 GHz. Simulation results are given in Fig.3, Fig.4 and Fig.5 for different D's, indicating the reflectance  $S_{11}$  apparently decreases with increasing the distance D.

This phenomenon can be obviously determined from the waveguide and the metal pins are the key parts of the simulation model [11]. We can use the electromagnetic software to optimize the dimensions of the waveguide, the radius of the metal pins, and the gas pressure in the simulation model[11].

## CONCLUSION

In this paper, we simulated the plasma discharge in three dimensions by COMSOL multi physics software

and proved that this simulation software is very powerful and very useful in different fields in science and technology. We simulated the EM-plasma interaction and microwave discharge in chlore inside a waveguide. The coupled EM-plasma system needs three studies and physics in COMSOL and coupled them by multi physics system in spite of this fact that my components were multiscale and multi physics[12]. Coupling these three physics, the chlore discharge waveguide problem was successfully simulated and the dominant physical mechanisms were accurately accomplished during the plasma formation process, which provides a deeper insight and better understanding of the physical phenomena and the plasma discharge details.

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