Comsol Multiphysics Application For Estimating Ozone Concentration in A Chamber With Plane Electrodes

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***Abstrak*- Berbagai kajian dan penelitian telah dilakukan terhadap pembangkitan plasma ozon menggunakan Metode *Dielectric Barrier Discharge* (*DBD*) dengan kondisi plasma non termal. Metode *DBD* memiliki berbagai keunggulan seperti distribusi medan listrik yang seragam pada penghalang dielektrik dalam menghasilkan plasma. Dalam studi ini, aplikasi COMSOL Multiphysics digunakan untuk melakukan pemeriksaan plasma ozon dari Ozone Chamber - yang terdiri dari elektroda plat aluminium berlubang dengan salah satu elektroda konfigurasi berlubang yang dipisahkan oleh dielektrik kaca tunggal. Perangkat lunak COMSOL Multiphysics memiliki Modul Plasma yang mencakup parameter elektrostatis, difusi *drift*, dan transportasi spesies berat untuk menghasilkan pelepasan pada O2 murni dengan keluaran konsentrasi ozon plasma. Dari hasil analisis simulasi diperoleh konsentrasi ozon tertinggi sebesar 3710,476 ppm pada tegangan masukan 8 kV dan konsentrasi terendah sebesar 3682,598 ppm pada tegangan masukan 5 kV. Hal tersebut menunjukkan bahwa tegangan yang diberikan pada elektroda memiliki korelasi linier dengan konsentrasi ozon yang dihasilkan.**

Kata Kunci- ozon, plasma, dielectric barrier discharge

***Abstract*- Various studies and research have been carried out on the generation of ozone plasma using the Dielectric Barrier Discharge (DBD) Method with non-thermal plasma conditions. DBD Method has various advantages such as the uniform distribution of the electric field on the dielectric barrier to producing plasma. In this study, COMSOL Multiphysics application was used to carry out ozone plasma examination from the Ozone Chamber – which is composed of a perforated aluminium plate electrode with a perforated configuration separated by a single glass dielectric. COMSOL Multiphysics software has a Plasma Module that includes electrostatic parameters, drift-diffusion, and heavy species transport to produce discharge on pure O2 with an output of plasma ozone concentration. From the results of this simulation analysis, the highest obtained ozone concentration was 3710.476 ppm at the applied voltage of 8.0 kV and for the lowest concentration was 3682.598 ppm at 5.0 kV applied voltage. It shows that the applied voltage to the electrode has a linear correlation with the generated ozone concentration.**

Keywords: ozone, plasma, dielectric barrier discharge

NOMENCLATURE

n_o : Number of initial electrons at initial distance
n_+ : Number of electrons when hitting the anode
n_e : Number of electrons when leaving the cathode
α : Townsend's first ionisation coefficient
d : gap distance
γ : Townsend's second ionisation coefficient
i : average current between gaps
e : exponential

I. INTRODUCTON

The generation of ozone using Dielectric Barrier Discharge (DBD) is considered the most optimum and effective method. In the DBD method, two electrodes separated by a dielectric material was utilised to produce non-thermal plasma at standard temperature and atmospheric pressure [1].

The application of DBD was developed by applying a high voltage to the electrodes coinciding with the dielectric layer and earthing the other electrodes. Ozone formed by spreading gas into the gap between the two electrode dividing walls that were triggering ionisation in the flowed gas through plasma discharge [2].

Plasma discharge was triggered by collisions between gas molecules and electrons. Meanwhile, the collisions were caused by the electric field between two parallel electrodes [3].

In previous studies [4], [5], for ozone generation, several things must be considered, namely the input voltage, chamber pressure, oxygen concentration and volume of the discharge chamber (chamber). According to research by Budiman et al. [6], the highest ozone concentration was obtained at 2979.9 ppm in a chamber using perforated aluminium electrodes with an electrode area of 99.58% at a voltage of 8 kV RMS. The ozone concentration at an input voltage of 8 kV is higher than at an input voltage below 8 kV. They show that the greater the input voltage, the greater the ozone concentration produced.

According to Sidik et al. [4] and Budiman et al. [5], the higher the input voltage, the greater the electric field formed so that the discharge that occurs more intense. Also, there are other studies on the generation of ozone using a chamber with various influenced factors including the electrical characteristics of the power supply, type of discharge, temperature, type of gas, and chamber pressure. Meanwhile, changing the power supply is considered as the right way to improve ozone generator performance [5]. Controlling some of these parameters can be applied in further research to produce an optimum ozone concentration.

In gas failure, there is a primary and secondary mechanism. In the primary mechanism, there is a flood of electrons due to collisions, ionisation due to light and heat. Then the plasma resulting from ionisation of a neutral gas generally contains an equal number of positive and negative charge carriers. Non-thermal plasma generally uses DBD as a medium for plasma formation because it has advantages including having a dielectric material that functions to distribute the electric field so that the discharges are formed evenly and uniformly in volume.

Besides, DBD could prevent spark formation due to the presence of dielectric material so that it has another name, e.g. silent discharge [3].

The current occurring between two parallel plate electrodes as a function of the applied field strength was first investigated by Townsend. When the voltage gradient that occurs is high enough, there are more electrons ionised than the number of ions that become the oxygen molecule, so that the electron pool leads to an opposite-charged plate and a collision occurs. More electrons are released, causing electron avalanches [1] .

In explaining the increase in current, Townsend introduces a factor α, known as Townsend's first ionisation coefficient. The definition of the factor α is the number of electrons in the path of an electron moving 1 cm in the direction of the field. Thus it can be written Eq. (1) and Eq. (2) for describing the condition for the increase in *dn* to the number of electrons *n* along with the *dx* [7]:

$$dn = \alpha n\, dx \tag{1}$$

$$n = n_o\, e^{\alpha x} \tag{2}$$

The number of electrons hitting or striking the anode per second as far as *d* from the cathode is equal to the number of positive ions as shown in Eq. (3):

$$n_+ = n_o e^{\alpha d} \tag{3}$$

The number of electrodes leaving the cathode and reaching the anode is shown in Eq. (4):

$$n_e = (n_o e^{\alpha d}) \,/\, (1-\gamma\,(e^{\alpha d}-1)) \tag{4}$$

Based on the literature, simulation studies on optimisation of the ozone chamber in producing ozone concentration are very limited. Therefore, research to simulate ozone concentration production by using advance software is essential to carry out. The previous chamber design by Budiman et al. has been selected to verify the simulation results.

II. METHODOLOGY

This study entirely using software, i.e., Solidworks, and COMSOL Multiphysics. Solidworks was used for modelling the chamber design in 3D. Solidworks has complete and user-friendly features as well as detailed image modelling. Meanwhile, simulation testing was carried out using COMSOL Multiphysics software which has several features for the research. After the modelling was complete, the geometry was imported to the COMSOL Multiphysics application via a 3D CAD file. This simulation computation used a computer with the operating system specification Windows 10 Pro for Workstations 64-bit (10.0, Build 1836.2).

A chamber based on previous research conducted by Budiman et al. was utilised [5]. This chamber is used to place electrodes with a predetermined arrangement, i.e., perforated electrode, dielectric, and perforated electrode. The perforated electrode materials were aluminium, with dimensions of 100 mm x 150 mm x 3 mm and cavities diameter of 1 mm. Meanwhile, the dielectric material used as a barrier was glass, which is a material commonly used as a barrier in the DBD system. The dielectric material has the same dimensions as the electrodes. Figure. 1 shows the shape of the chamber used for ozone generation.

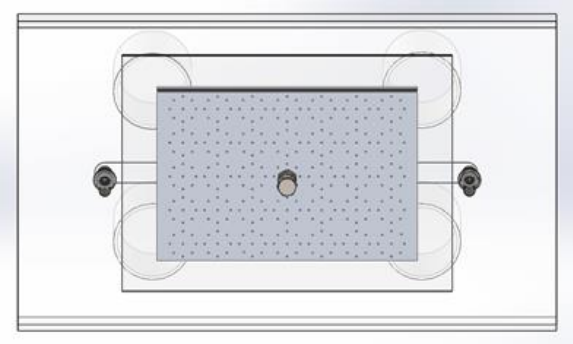

Fig. 1. Ozone chamber

A. Chamber Simulation Modelling Design

In testing, the chamber modelling design used is the component that affects the results of ozone concentration fundamentally, namely electrodes, glass, and air models. In modelling, the glass and air were made to the same size as the electrodes. The outlet and inlet sections in the modelling were adjusted to the boundary conditions of the plasma test geometry. Figure 2 and Figure 3 shows the chamber components.

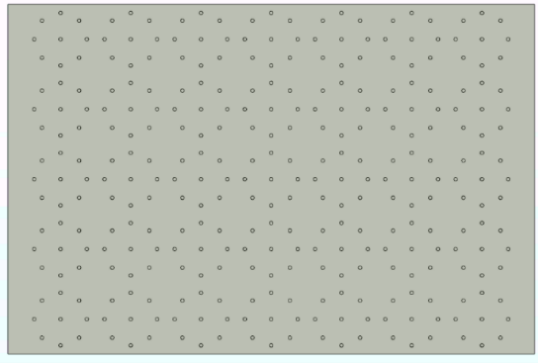

Fig. 2. Chamber components required for simulation – Top View

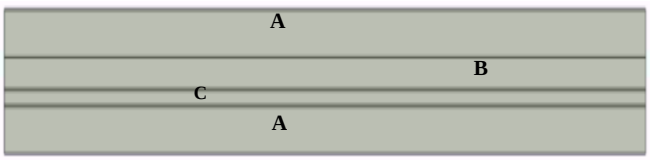

Fig. 3. Chamber components required for simulation – Side View (A: perforated aluminium, anode-cathode; B: glass; C: Gap).

B. Simulation Boundary Conditions

In the simulation, a geometric model was prepared and adjusted to the simulation state through boundary conditions. The boundary conditions of the simulation were based on the physical parameters applied to each component of the chamber, the electron and plasma transport properties. Figure. 3 shows the high voltage (HV) supply was AC voltage; thus, the upper electrode used the voltage versus time equation. Dielectric and electrode materials were conditioned by entering the physical properties of the material such as relative

permittivity, electrical conductivity, and thermal conductivity. In this study, a distance of 1 mm was used as a wall for plasma formation and a domain for gas flow. The outlets and inlets in this modelling were conditioned on the boundary of the right and left air walls.

The input gas used was pure O2 with the initial mole fraction considered 1. The situation around the chamber was 293.7 K and a pressure of 1 atm. The oxygen gas temperature setting was 300 K following the state of the plasma non-thermal conditions and gas discharge settings in the Phelp database used. The boundary conditions are shown in Figure 4.

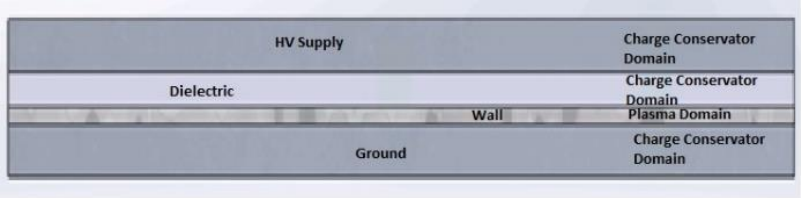

Fig. 4. Simulation boundary conditions for ozone plasma generation.

III. RESULTS AND DISCUSSION

This plasma modelling used pure O2. The computational discharge model includes the ionisation of electrons from ionic species. In the discharge process, various rotational collisions and vibrations were considered in the electron energy equation. The reaction as a discharge process included mechanisms such as elasticity, attachments, and ionisation were assessed through electron collision data in the E/N function of the electron impact reaction. This electron reaction coefficient as a function of the reduced electric field was expressed in Td. Td is the physical unit of the E/N ratio, where E is the electric field (V/m), and N is the concentration of neutral molecules ($1/m^3$).

The formation of a plasma in this simulation takes data with a local field approximation by reducing the electric field. When the electrode is subjected to a voltage, it will cause an electric field. The electric field produces a collision between molecules in the gas and electrons, causing failure of O2. Current flows between the walls of the gap due to the failure. The ionisation process was initiated, and discharges occur lead to plasma formation. In this condition, the oxygen molecule becomes atomic oxide (O) which occurs as a result of the reaction of oxygen with electrons in an electric field so that the O atom combines with oxygen and produces O3 (ozone). Electric fields on sharp or tapered surfaces will cause a corona discharge so that the perforated part of the electrode – covered by the dielectric – will cause more O2 ionisation to become ozone.

The ozone plasma simulation results are displayed in two voltage states. First, the state of the AC voltage is adjusted according to the experiment. This simulation was carried out in five periods of 0.1 s with 0.02 s periodic. In this simulation, the input voltage uses the general sinusoidal function (V (t)) with a fixed frequency of 50 Hz. Table I shows the ozone concentration results.

TABLE I. OZONE CONCENTRATION RESULTS ON AC VOLTAGE CHAMBER.

No	Vin (kV)	Vp (V)	Output Ozone (mol)	Output Ozone (ppm)
1.	5	7071	4.05932×10^{-7}	3682,598
2.	6	8485	4.07092×10^{-7}	3693,139
3.	7	9899	4.08026×10^{-7}	3701,606
4.	8	11313	4.09003×10^{-7}	3710,476

The second state used DC voltage input to see the conditions at the peak voltage. In the simulation using DC voltage, the computation was carried out the same as the AC voltage state, five periods of 0.1 s with 0.02 s periodic. However, the observation was carried out at the peak voltages (Vp). Table II shows the ozone concentrations.

TABLE II. OZONE CONCENTRATION RESULTS ON DC VOLTAGE CHAMBER.

No	Vin (kV)	Vp (V)	*Output Ozone* (mol)	*Output Ozone* (ppm)
1.	5	7071	4.06197×10^{-7}	3685,017
2.	6	8485	4.07446×10^{-7}	3696,336
3.	7	9899	4.08123×10^{-7}	3702,499
4.	8	11313	4.10477×10^{-7}	3723,840

The results show that higher voltage produces higher ozone concentration. The products of ozone concentration tend to be larger but stable on the DC input voltage. This indicates that the discharge current at the DC input voltage is more generous than the AC input voltage, which causes more electrons to be produced and more massive plasma excitation.

However, the stability of the results of the ozone concentration of the two simulations is due to the reduction of the same electric field by COMSOL Multiphysics computation through the cross-section of pure O2 discharge data and the same maximum input voltage in each of the AC and DC voltage equations. So that the resulting maximum field rectification is the same even though with a different local field approach process.

In order to verify the simulation results, a comparison with experimental results has to be carried out. The simulation results are compared with Budiman et al. [5] results that show in Figure 5.

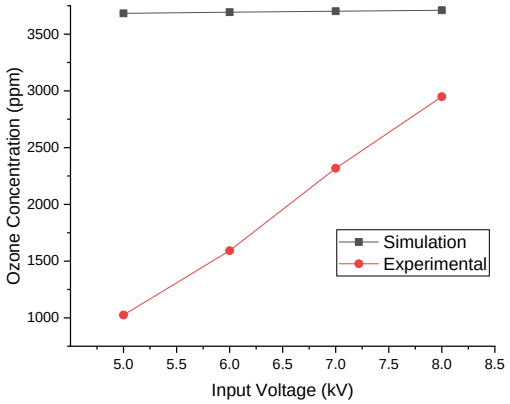

Fig. 5. Comparison graph of ozone concentration results, simulation and experimental.

Figure 4 shows, in the simulation, the ozone concentration increment against input voltages is less significant compared to the increment of experimental results. However, the ozone concentration from the simulation is higher than the experimental. Table III presents a detailed comparison of ozone concentration.

TABLE III. COMPARISON OF OZONE CONCENTRATION RESULTS ON SIMULATION TEST WITH PREVIOUS EXPERIMENTS.

No.	O_3 concentration	
	Simulation (ppm)	Experiment (ppm)
1	3682,598	1024,830
2	3693,139	1592,430
3	3701,606	2317,700
4	3710,476	2948,370

The difference between both – simulation and experimental – due to no losses occurred in the simulation. Several potential losses are voltage loss on the electrode, ozone concentration deficiency along transmitted to ozone measuring instrument, and decomposition of the ozone reaction against the electrode wall.

IV. CONCLUSION

The chamber design and simulation have been carried out by using Solidworks and COMSOL Multiphysics to observe the ozone concentration produced based on the previously developed chamber and experimental results. The simulation results verified by the experimental results show that voltage input has a contribution to ozone concentration production

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