doi:10.14311/ppt.2024.3.54
Plasma Physics and Technology **11**(3):54–60, 2024

STUDY OF ELECTRIC FIELD DISTRIBUTION ON PLASMA AND PLASMA CATALYSIS REACTOR FOR DIFFERENT ELECTRODE CONFIGURATIONS AND PELLET SIZES

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Abstract. In various non-thermal plasma-based applications, the dynamics of electric fields and charged particle interactions are crucial. In order to find an efficient plasma reactor, the effects of different electrode configurations for the plasma approach and pellet packaging & optimal sizing for the plasma catalysis approach were studied for 5 different types of volume discharge and surface discharge reactors using COMSOL Multiphysics 6.0. The different electrode configurations, viz., concentric cylindrical, square, and helical as volume-discharged reactors and floating & 2 types of non-floating electrodes as surface discharge rectors, are considered. The effect of different size (diameter 1/3/5) of pellets was studied for helical and cylindrical plasma reactors for plasma catalysis.

Keywords: Non thermal plasma, plasma catalysis, COMSOL Multiphysics 6.0, diesel engine exhaust treatment, pellet size, plasma electrode configurations.

1. Introduction

The application of non-thermal plasma (NTP) technology is revolutionizing the cleanup and pollution control of our surroundings. Chemical reactions are triggered without the requirement for extremely high temperatures by means of certain gases that have been converted into electrically charged particles. These reactions can be used to aid in the breakdown of pollutants, leading to cleaner air and water. Nevertheless, a thorough understanding of the behavior of charged particles and electric fields inside the plasma-generating machinery is essential to the optimal functioning of NTP [1].

In this study, we take a close look at different ways of setting up these machines, which are called plasma reactors. There is an important type of reactor called a dielectric barrier discharge (DBD) reactor, which is commonly used in NTP technology. It has been trying out different shapes and arrangements of electrodes inside these reactors to see which ones work best. It is also experimenting with new kinds of electrodes that float in the air instead of being connected to the ground. This might change how the plasma behaves.

Additionally, it is investigated how adding small pellets of certain materials into the reactor can affect the way the electric fields are spread out. This is important because it can change how well the reactor can clean up exhaust gases from diesel engines, which produce harmful pollutants like nitrogen oxides NO_x. By testing different sizes of these pellets and seeing how they affect the reaction, it is hoped to figure out the best way to make the reactor work even better [2].

NTP is made when really strong electric fields are created that excite the gases inside the reactor. This can happen in different ways, like with DBD or Corona discharges. DBD is especially good for making NTP because it works at regular air pressure and room temperature. It's been used for lots of things, like cleaning water, sterilizing things, and even making ozone, which can help clean the air. When we make NTP with DBD, it happens because the electric field is strong enough to make a kind of spark called a streamer. This streamer makes a mix of positive and negative charges in the gas that we call plasma. This plasma can help break down pollutants in the air or water [3].

The experiments have shown some interesting results. It is found that one particular electrode setup, called a helical electrode, seems to make the strongest electric fields inside the reactor. This means it could be really good at cleaning up pollution. It has also been discovered that using certain-sized pellets can make a big difference in how well the reactor can clean up exhaust gases. For example, using pellets that are 5 mm in diameter seems to work best for certain types of reactors [4, 5].

The overall goal of the research is to improve the environmental cleansing capabilities of NTP technology. By being aware of the ways in which various reactor configurations and pellet sizes impact the procedure.

In conclusion, this work represents a significant advancement in the use of NTP for pollution management and environmental cleanup. by determining how to improve the behavior of the electric fields inside the reactors.

2. Experimental Set-up

The complexity of plasma chemistry, with its diverse variety of timing features, reactions, and products,

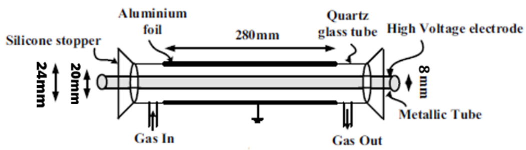

Figure 1. Schematic diagram of the reactor

presents a problem when it comes to computational challenges and expensive simulations when it comes to modeling and simulation.

Plasma chemistry involves a number of computing tasks due to the microsecond-scale nature of the ionization, recombination, de-excitation, and excitation processes. Because of this, the majority of 1-D plasma models found in the literature are designed to minimize computing time and expense [1].

2.1. Volume Discharge

The 3-D model's geometry features include the following: The dielectric (quartz) tube has an outer radius of 12 mm and a thickness of 2.0 mm. The *HV* electrode is a stainless steel cylinder with a radius of 4.0 mm and a length of 300 mm [1]. The ground electrode is made of aluminum and spans 280 mm of the tube's length in the middle and at its outer circumference. Air has a relative permittivity of 1.0, whereas quartz has a value of 4.2. Fig. 1 presents the schematic diagram of the reactor, and Fig. 2 demonstrates the designed 3-D geometry of the reactor in COMSOL.

Applying a high voltage to the inner electrode causes a strong electric field to form in the area between the two electrodes. This electric field goes from the high-voltage electrode to the ground electrode. On application of a 25 kV ac voltage at a frequency of 50 Hz, the electric field's direction also changes simultaneously.

The strong electric field provides enough energy to liberate electrons and start ionization processes. In the opposite direction of the electric field, these freshly created electrons travel in the direction of the boundary surfaces. An equivalent number of positively charged particles, or ions, are moving in the same direction at the same moment. Five distinct electrode designs are available: solid cylindrical, hollow cylindrical, square shape, helical shape, and a helical wire mounted on a square-shaped electrode [6].

2.2. Surface Discharge

Surface dielectric barrier discharge, or SDBD, is a type of gas discharge phenomenon that occurs when an electric field is applied to the surface of a dielectric material, such as glass or ceramic. Starting and sustaining this discharge depend on the strength of the electric field. An SDBD is typically initiated by applying a high-voltage electric field to the dielectric

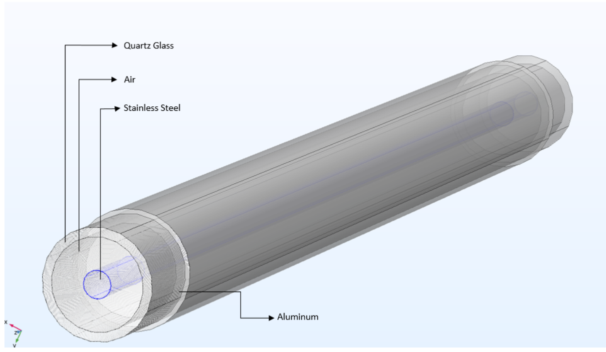

Figure 2. COMSOL model reactor 3-D geometry for solid cylindrical electrode

surface. Because of the dielectric material, the discharge occurs at or near the dielectric surface rather than directly between the electrodes [6]. When the electric field intensity surpasses a certain threshold, also known as the breakdown voltage, the dielectric material degrades, and a plasma discharge may occur at the surface. The intense electric field ionizes the nearby gas molecules.

Fig. 3 demonstrates the designed COMSOL 3-D geometry for surface discharge. A glass plate of 80 mm in length and 10 mm in breadth has copper metal strips affixed to it, each measuring 8 mm in width and 0.5 mm in thickness. An aluminum ground electrode is attached to the back of the glass panel. An additional piece of aluminum ground has been attached to the upper surface of the glass plate, 4 mm from the lower glass plate. Plasma is created in the area between these two plates. A 50 Hz, 25 kV ac voltage is applied to the alternating metal electrode, leaving the other electrodes floating. There are primarily two configurations: non-floating and floating surface discharge [7].

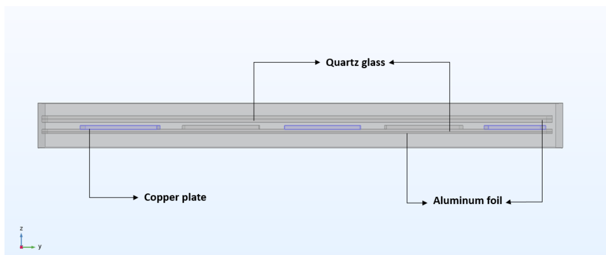

Figure 3. COMSOL model: Reactor 3-D geometry for surface discharge

2.3. Volume Discharge with Pellets as Catalyst

This study examines the effectiveness of using pellets as catalysts to improve the removal of NO_x emissions from diesel engine exhaust and other combustion processes using dielectric barrier discharge (DBD) models. Fig. 4 demonstrates the schematic diagram of the reactor with pellets of different sizes. The objective is to speed up the physical and chemical processes in

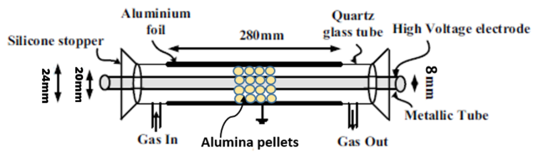

Figure 4. Schematic diagram of the reactor with pellets

the plasma reactor. In order to enhance NO_x removal effectiveness and optimize catalytic activity, this technique explores a number of parameters, including pellet size and material composition [6, 7].

This research contributes to ongoing efforts to develop more effective technologies for mitigating air pollution and improving public health. Fig. 5 demonstrates the designed COMSOL 3-D geometry for volume discharge with pellets. Stainless steel electrodes with a cylindrical or helical shape are the two most common electrode configurations. The pellets that are used are 1 mm, 3 mm and 5 mm in size. The pellets are inserted into the plasma reactor's center, measuring 30 mm in length. The dielectric tube is made of quartz glass and measures 300 mm in length, and the ground electrode is 280 mm in length [8].

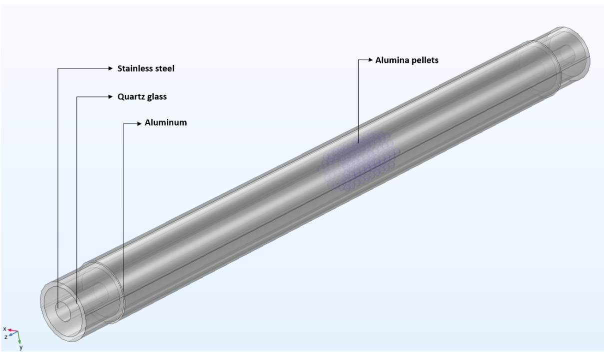

Figure 5. COMSOL model: Reactor 3-D geometry for volume discharge with pellets size $d = 3$ mm

3. Governing Equations

3.1. Gauss's Law

In this section, provide a concise overview of the electrostatic physics governing equations employed in the COMSOL simulation. Equations describing the basic interactions between charged particles and neutral gas molecules, as well as the electric field and charged particles, are found through numerical analysis of the model.

The formulations utilized in this study are grounded in Gauss's law [1]. Gauss's law describes the relationship between the electric field ($\mathbf{E}$) and the charge density (ρ). The equation is given by:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{1}$$

where:

- $\nabla \cdot \mathbf{E}$ is the divergence of the electric field,
- ρ is the total volume charge density,
- ε_0 is the permittivity of free space.

The electric displacement ($\mathbf{D}$) involving free charge:

$$\nabla \cdot \mathbf{D} = \rho \tag{2}$$

For linear materials, where $\mathbf{E}$ is directly proportional to $\mathbf{D}$:

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_0 \varepsilon_r \mathbf{E} \tag{3}$$

For nonlinear materials, where $\mathbf{D}$ is expressed as the sum of linear and nonlinear components:

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E} + \mathbf{D}_r \tag{4}$$

The displacement in the absence of an electric field is represented by the remnant displacement $\mathbf{D}_r$. Boundary conditions must be taken into account in order to arrive at a unique solution. The following equations express these conditions, which characterize the interaction between various media:

$$\hat{n}_2 \cdot (\mathbf{D_1} - \mathbf{D_2}) = \rho_s \tag{5}$$

where the outward normal from medium two, which is dielectric in this instance, is represented by $\hat{n}_2$.

3.2. Calculation for Optimal Diameter (d_{opt})

A theoretical computation is performed to determine the ideal diameter d_{opt}. The discharge power is at its highest when the pellet diameter d_{opt} is at its optimal value. Reactor capacitance decreases with d bigger or smaller than d_{opt}, lowering discharge power [5].

Theoretically, $d_{\text{opt}} = 2.54$ mm; however, $d_{\text{opt}} = 3$ mm is used to reduce computational complexity.

3.3. Poisson's Equation

In the context of plasma discharge in a volume, Poisson's equation plays a crucial role in describing the electric field distribution within the plasma. Poisson's equation is a partial differential equation that relates the electric potential to the charge distribution in the plasma [1].

The electric field's divergence is $\nabla \cdot \mathbf{E}$. The charge density is ρ, and the electric field is $\mathbf{E}$. Free space permittivity is ε_0.

Applying the divergence operator to both sides of Gauss's law, we obtain:

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0} \tag{6}$$

Here, ϕ represents the electric potential. The expression $\nabla^2 \phi$ is the Laplacian of the electric potential, often denoted as $\nabla^2 \phi$ or $\nabla^2 V$, where V is the electric potential [4].

The contribution of both free charges (electrons and ions) and any fixed charges (e.g., ions bound in the lattice of solid electrodes, if present) is included in the charge density ρ in the plasma discharge.

$$\mathbf{E} = -\nabla\phi \tag{7}$$

Solving Poisson's equation allows us to determine how the electric potential varies throughout the plasma volume due to the distribution of charges. The electric field can then be obtained by taking the negative gradient of the electric potential.

4. Simulation Results and Discussion

The AC/DC module of COMSOL Multiphysics was utilized for conducting investigations through the Electrostatics interface. Chemical reactions were not taken into account in the three-dimensional (3-D). The flow rate of seven liters per minute is used in laminar flow physics. During the simulation, a voltage of 25 kV domain-wise at $f = 50$ Hz with time dependency was applied to the high voltage *(HV)* electrode [6].

A dielectric barrier discharge (DBD) plasma reactor in the form of a cylindrical model was depicted. A cylindrical glass tube that served as a dielectric barrier encircled the axial high-voltage *(HV)* electrode that made up the reactor. The outside edge of the dielectric was covered with a ground electrode. The axial *HV* electrode and the inner surface of the dielectric were filled with air, which was used to create non-thermal plasma.

The rms value of the electric field is calculated for a volume discharge-based reactor using volume integration and equation

$$E_{\text{rms}} = \sqrt{E_x^2 + E_y^2 + E_z^2} \quad (\text{V*m}^2) \tag{8}$$

4.1. Volume Discharge

The simulation resulted in a greater average electric field in the helical electrode configuration, solid cylindrical electrode configuration, and so forth. In this study, efforts have been made to find the maximum electric field to exhibit the effect of electrode shape and discharge type.

Fig. 6 demonstrates the distribution of electric field (V/m) in a cylindrical electrode. The maximum electric field measured from the solid and hollow cylindrical electrode configurations is 6.45 MV/m, whereas the helical electrode configuration, which exposed the plasma reactor's inner surface, produced an maximum electric field of 102.40 MV/m [1, 7].

Fig. 7 demonstrates the distribution of electric field (V/m) with helical electrode configuration. The helical electrode arrangement has the highest rms electric field in the volume.

The helical wire mounted on a square-shaped electrode has the highest electric field strength at the corners. In specific places, the electric field intensity can increase significantly due to sharp edges or corner, such as a needle or a pointed wire, followed by the square-shaped electrode. Fig. 8 shows the distribution

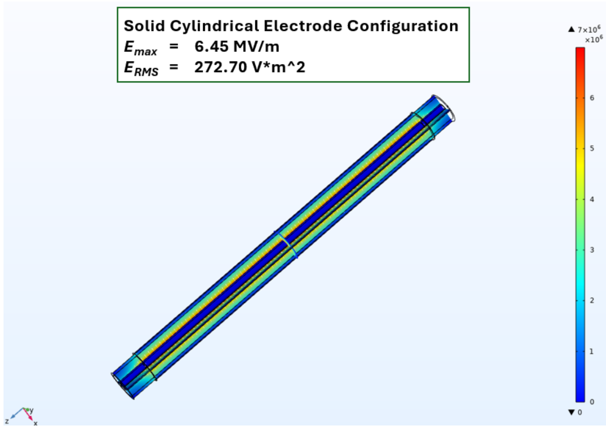

Figure 6. Distribution of electric field (V/m) with solid cylindrical electrode configuration

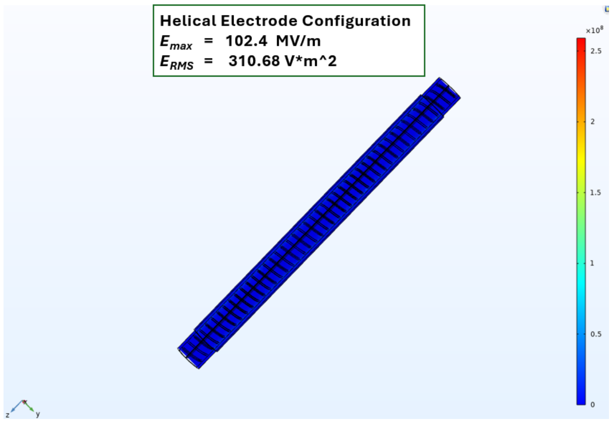

Figure 7. Distribution of electric field (V/m) with helical electrode configuration

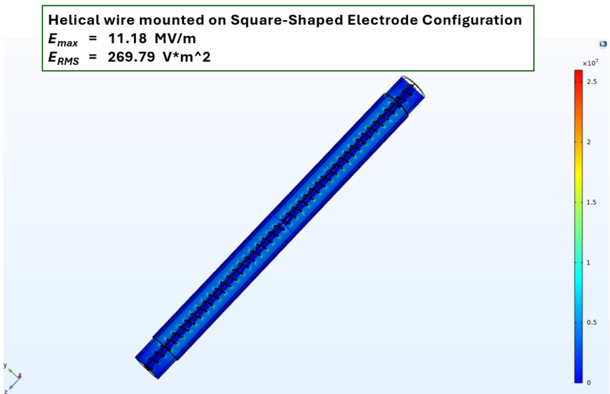

Figure 8. Distribution of electric field (V/m) with helical wire mounted on a square-shaped electrode

of electric field (V/m) for this arrangement. Around corners or edges, the electric field intensity increases due to a process called "charge concentration".

4.2. Surface Discharge

In a surface discharge setup with two electrode configurations, one with a floating electrode and the other with a non-floating electrode, the behavior of the discharge can vary significantly. When a high voltage

Electrode Shape	Rms $(V*m^2)$	Emax (MV/m)
Helical Shaped Electrode	310.68	102.4
Hollow Shaped Electrode	274.43	6.18
Solid Cylindrical Shaped Electrode	272.70	6.45
Helical wire mounted on a Square-Shaped Electrode	267.07	11.18
Square Shaped Electrode	250.13	7.42

Table 1. Electrode shapes with corresponding Rms and Emax values

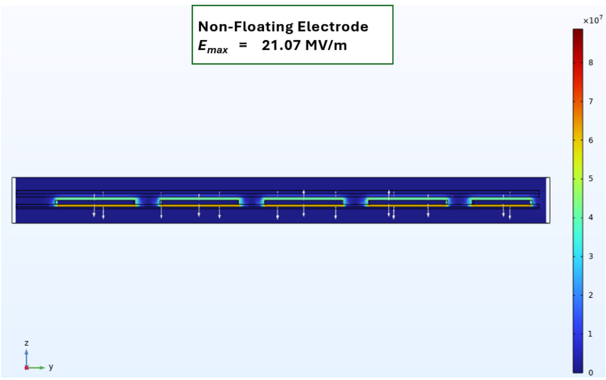

Figure 9. Electric field (V/m) at the surface of non-floating electrode

(25 kV ac, 50 Hz) is applied, a surface discharge may occur between the electrodes depending on factors such as the gap distance, gas composition, and surface conditions.

4.2.1. Non floating electrode

All five metal strips are connected to the *HV* supply. The rms electric field on the surface we examined is 19.37 MV/m.

The cross-sectional view of the electric field distribution (MV/m) at the surface of the non-floating electrode is shown in Fig. 9. A powerful electric field is created surrounding the floating electrodes when a high voltage is applied to them. Ionizing the surrounding gas at a high enough voltage can result in the production of plasma. Surface treatment or modification may result from this plasma's subsequent interactions with the materials or surfaces in the vicinity.

Fig. 10 demonstrates that electric field lines tend to converge near sharp edges or corners of a surface, which results in a concentration of electric field intensity. The electric field lines, which depict the path a positive test charge would travel, are blocked and twisted around the curve [3, 9].

4.2.2. Floating electrode

The rms electric field measured on the surface, 11.33 MV/m, indicates the strength of the electric

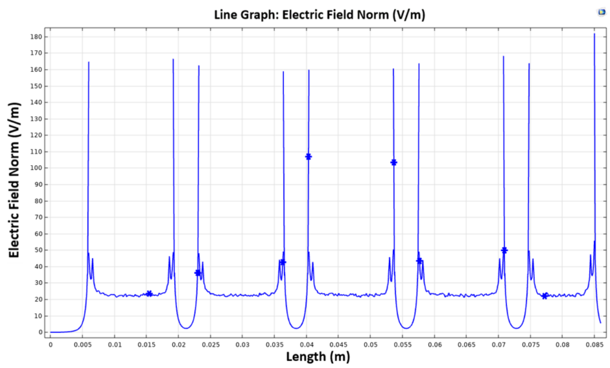

Figure 10. Result of electric field (V/m) simulation on the surface of non floating electrode configuration

field encountered on the material's surface, where the floating electrodes are situated.

As seen in Fig. 11, the charge density is spread unevenly due to the abrupt discontinuity of the electric field caused by the sharp corners. When compared to a non-floating electrode, the floating electrode has a lower average electric field norm because the copper strips are linked to the high voltage *(HV)* infrequently. This configuration probably has an impact on the system's electric field strength and distribution [7].

Fig. 12 demonstrates the electric field (V/m) at the surface of the floating electrode.

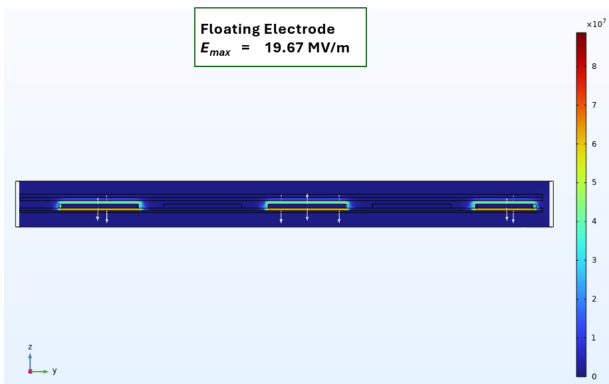

Figure 11. Electric field norm (V/m) along the length of floating electrode

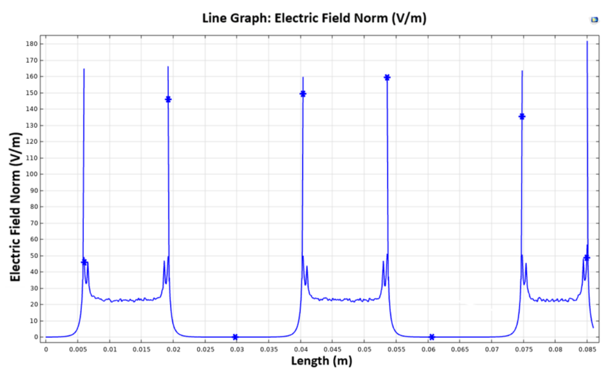

Figure 12. Result of electric field (V/m) simulation on the surface of floating electrode configuration

4.3. Volume Discharge with Pellets

4.3.1. Cylindrical electrode with different pellets size

The distribution of the electric field on the surface of the pellets and inside the voids, or spaces between the pellets, is a crucial component in determining the reactor's efficiency. Alumina is the material of the pellets that are used, and stainless steel is the material of the cylindrical electrode.

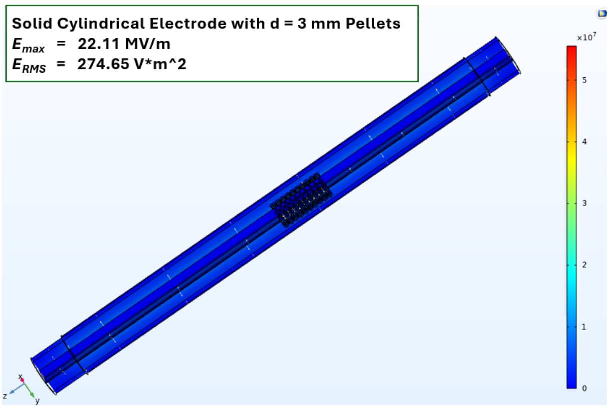

Figure 13. Cylindrical electrode simulation result for electric field (V/m) with pellets of size $d = 3$ mm

The geometry of the electrodes, their spacing, and, if applicable, the dielectric properties of the medium govern the distribution of the electric field in the gaps between the pellets. Different particle sizes can have an effect on how the electric field is distributed in the voids. Due to the shortened distance between opposing charges on the electrodes, smaller pellets may enable closer spacing between electrodes, which could result in stronger electric fields [10].

The electric field (V/m) simulation result for pellets with a dimension of 3 mm is shown in Fig. 13. It can be unfavorable to experience arcing or electric field saturation between electrodes if the separation is too tiny.

The rms electric field in volume for the $d_{\text{opt}} = 3$ mm is 274.65 V*m^2. The rms electric field of $d = 1$ mm is 273.10 V*m^2, and the rms electric field of $d = 5$ mm is 272.85 V*m^2, which come next. Thus, the cylindrical electrode with $d_{\text{opt}} = 3$ mm will produce the largest rms electric field value in the volume.

Pellet Size (d)	Rms (V*m^2)	Emax (MV/m)
$d = 1$ mm	273.10	33.47
$d = 3$ mm	274.65	22.13
$d = 5$ mm	272.85	10.22

Table 2. Cylindrical electrode with different pellet sizes

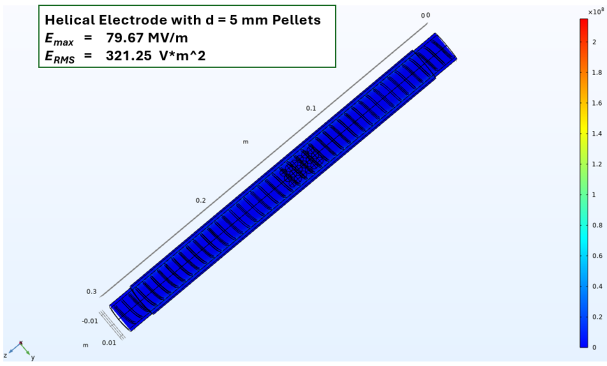

Figure 14. Helical electrode simulation result for electric field (V/m) with pellets of size $d = 5$ mm

4.3.2. Helical electrode with different pellets size

Compared to conventional linear electrodes, this arrangement provides a greater surface area, which can boost plasma formation and enhance reactor performance as a whole. In order to achieve consistent plasma formation across the reactor volume, the helical design also helps to create a more uniform electric field distribution throughout its length.

Adding different-sized pellets to the helical electrode arrangement complicates the kinetics of plasma formation and the dispersion of the electric field. Smaller pellets might make it possible to pack the helical structure more tightly, which could increase the density of discharge sites and improve the efficiency of plasma formation. On the other side, larger pellets might have larger surface areas, which could result in better interactions with the plasma and possibly affect its overall properties [10].

Fig. 14 demonstrates the electric field (V/m) simulation result for pellets size $d = 5$ mm. For $d = 5$ mm, the rms electric field in the volume is 321.25 V*m^2. For $d = 3$ mm, the rms electric field is 312.27 V*m^2, and for $d = 1$ mm, it is 309.17 V*m^2. The distribution of electric fields obtained with the 5 mm-diameter pellet appears to be appropriate for supporting effective plasma formation within the NTP reactor, based on the observed trend in rms electric field strengths in the volume.

The 5 mm diameter pellet surface has a greater average electric field strength, which promotes more efficient breakdown of the surrounding gas and increases plasma formation and sustained discharge.

4.3.3. Void percentage

Variations in the void percentage can have an impact on the distribution and concentration of electric fields inside the cylindrical reactor [10].

The ideal diameter for the cylindrical electrode arrangement is $d = 3$ mm, at which the void% is 26.25% and the electric field intensity is at its maximum. This implies that the ideal diameter layout makes it easier for electric fields to be generated and concentrated inside the system.The electric field strengths are somewhat lower for both the larger $d = 5$ mm

Pellet Size (d)	Rms (V^*m^2)	Emax (MV/m)
$d = 1$ mm	309.17	31.8
$d = 3$ mm	312.27	26.83
$d = 5$ mm	321.25	79.88

Table 3. Helical electrode with different pellet Sizes

void% of 49.33% and the smaller $d = 1$ mm void% of 31.83%. This implies that when there are deviations from the ideal diameter, the electric fields become slightly weaker.

In the helical electrode configuration, the void% for $d = 5$ mm is 25.33%, whereas the void% for $d = 1$ mm is 30.46% and the void% for $d = 3$ mm is 27.25%. The electric field reduces as the pellet size diameter lowers since it is largest at $d = 5$ mm, the optimum diameter. Thus, the void % was a critical aspect in establishing optimal electric field formation [3, 10]. The helical electrode with pellets of 5 mm diameter exhibits a maximum rms electric field of 321.25 V^*m^2 when compared to other reactors.

5. Conclusion

The major inferences drawn in the present study are as follows:

1. The helical electrode performs better for volume discharge with an rms value of electric field in volume is 321.25 V^*m^2.

2. Floating electrodes provide better control, but non-floating electrodes produce a more desirable surface discharge.

3. The solid cylindrical electrode with a particle size of $d = 3$ mm has the greatest rms electric field among the different pellet sizes with the solid cylindrical electrode and the lowest percentage of voids.

4. The helical electrode with $d = 5$ mm pellet size generated the greatest rms electric field among the different pellet sizes with the helical electrode, highlighting the significance of geometry and void percentage in demonstrating an improved electric field.

5. One of the most important factors in determining the ideal electric field generation in the plasma catalysis approach was the void percentage. A lower void percentage generates a higher electric field.

Finding the best reactor design can be aided by the knowledge and design ideas found in this study. However, more research utilizing a plasma module is required, taking into account both the electrostatics and the chemistry of the plasma.

6. Acknowledgement

Authors acknowledge the funding support provided by SERB Power SPG/2021/003513, Govt. of India.

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