

Article

Partial Discharge Simulation of Air Gap Defects in Oil-Paper Insulation Paperboard of Converter Transformer under Different Ratios of AC–DC Combined Voltage

Bing Luo ¹, Jian Wang ², Dong Dai ^{2,*} , Lei Jia ², Licheng Li ² and Tingting Wang ¹

¹ China Southern Power Grid Research Institute Co., LTD, Guangzhou 510663, China; luobing@csg.cn (B.L.); wangtingting@csg.cn (T.W.)

² School of Electric Power, South China University of Technology, Guangzhou 510641, China; 201920113422@mail.scut.edu.cn (J.W.); jialei@csg.cn (L.J.); lilc@csg.cn (L.L.)

* Correspondence: ddai@scut.edu.cn; Tel.: +86-10-8711-0613

Abstract: A converter transformer is important primary equipment in a DC transmission project. The voltage on the valve side winding is complex when the equipment is running, including DC, AC, and AC–DC combined voltage. The insulation structure of the valve side winding of a converter transformer is an oil-paper insulation structure, which may have a variety of defects in the manufacturing stage and daily use, resulting in partial discharge. Therefore, it is the key to studying the partial discharge characteristics and mechanism of oil-paper insulation under AC–DC combined voltage. In this paper, we build a two-dimensional air gap model of oil-paper-insulated pressboard considering the actual particles and actual reaction based on the fluid model. The characteristics and evolution mechanism of partial discharge (PD) in pressboard under different AC/DC combined voltages are studied by numerical simulation. The results show that when the DC component increases, the polarity effect of partial discharge is more obvious, while the potential and discharge intensity in the air gap decrease. Further analysis revealed that the DC component in the combined voltage accumulated a large number of surface charges on the surface of the air gap, and the space charge distribution was more uniform and dispersed, which generated an electric field with opposite polarity to the DC component in the air gap and, then, inhibited the development of local discharge in the paperboard. The results of the simulation are consistent with the previous experimental phenomena, and the mechanism analysis of the simulation results also verifies the previous analysis on the mechanism of experimental phenomena. This will lay a theoretical foundation for the further study of partial discharge phenomenon of oil-paper insulation structures in practical operation in the future.



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1. Introduction

In recent years, with the development of DC transmission projects, the voltage level of UHV DC in China has increased year by year, which has played an important role in solving the problems of large-capacity and long-distance transmission in China. Many scholars have carried out a lot of research on the stable operation and optimization of the UHV AC/DC system. Wang Weiyan combined the PSCAD component library with an e-tran model to simulate the operation characteristics and AC/DC interaction mechanism of an 800 kV DC transmission. This simulation model improves the accuracy of an electromagnetic transient simulation of an AC/DC power grid. Zhao Liying proposed a new power flow calculation method to analyze the voltage stability of VSC-HVDC AC/DC system, and the system has showed that the algorithm has good applicability and robustness [1–3].

In addition, the reliable operation of electrical equipment such as a converter transformer is also of great practical significance for HV-AC/DC transmission. Different from the traditional AC transformer, the oil-paper insulation structure of the converter trans-

former bears more complex voltage in actual operation, including DC, AC, and AC/DC superposition. There are great differences in the characteristics and mechanism of partial discharge under different voltage forms. Based on this, it is of great practical significance to study the characteristics and evolution mechanism of partial discharge under an AC/DC composite voltage to maintain the safe operation of the HVDC system [4–12].

At present, there are many experimental studies and reports on the partial discharge of an oil-paper insulation structure under AC–DC combined voltage. By building a simple oil-paper insulation structure model in the laboratory, scholars found that with an increase in the proportion of the DC component in the combined voltage, the initial voltage of the partial discharge increased, and the discharge repetition rate and the discharge magnitude decreased [6–10]. Furthermore, Chen Qingguo, Sha, and Li carried out a preliminary simulation of electric field and potential distribution under combined voltage by using finite element analysis software and circuit simulation, respectively. Combined with the previous experiments, they analyzed the mechanism of the experimental phenomenon: due to the existence of the DC voltage component in the combined voltage, a lot of surface charges and space charges are generated in the air gap, thus forming an electric field with opposite polarity to the DC voltage component and inhibiting the occurrence of partial discharge, but this analysis has not been clearly verified [13].

It can be seen that the current research in converter transformers has mainly been carried out in the laboratory environment by applying combined voltage to a simple oil-paper insulation model. Based on the experimental phenomena, scholars have analyzed the physical mechanism of partial discharge under combined voltage, but the analysis is still at the phenomenon level and cannot describe the microphysical process of partial discharge in the air gap. Sha simulated the oil-paper insulation structure, but the overall model is relatively simple and failed to reveal the microphysical evolution process of partial discharge in the air gap [13–20].

In recent years, with the improvement of the performance of supercomputers, computational high-voltage engineering has been proposed, which uses applied mathematics and computer science to solve or explain practical problems in high-voltage engineering. Computational high-voltage engineering is a supplement and development based on the traditional high-voltage experiment and research methods [12,13]. However, at present, the discipline of high-voltage engineering is still dominated by experiments, supplemented by empirical formulas and semi-physical models to explain high-voltage physical phenomena. For example, most of the traditional partial discharge models are three capacitance models and induced charge models. Although these models are helpful for qualitatively understanding the surface phenomenon of partial discharge, their physical meaning is not strictly clear. After considering the shortcomings of the traditional partial discharge model, Callender et al. proposed a virtual ionic fluid model based on the plasma dynamic process in partial discharge. The model describes the physical processes such as the migration, diffusion, and recombination of electrons and ions [21,22], which is of great significance to the study of the mechanism of partial discharge.

However, the model built by Callender does not consider the actual chemical particles and reactions. Therefore, we have developed a plasma partial discharge model considering more than 20 kinds of actual particles and their chemical reactions in the air gap. The model enables us to explain the physical mechanism of partial discharge behavior from the perspective of physicochemistry and observe the accumulation and decomposition of chemical substances in partial discharge [21–28]. In this paper, we use this model to understand the evolution mechanism of partial discharge of an oil-paper insulation structure under combined voltage more deeply and accurately.

2. Model and Simulation

2.1. The Air Gap Model of Insulating Pressboard

There are often residual air bubbles in the manufacture of a converter transformer and the solidification and decomposition of organic materials. Besides, although vacuum

drying and impregnation techniques are usually used, mechanical stress can cause local cracks [17]. These internal air gaps accelerate the aging of an oil-paper insulation structure. Partial discharge in the internal air gap of insulating materials is considered one of the main causes of insulation breakdown.

In the model, the relative dielectric constant of the air gap ε_1 inside the insulating medium is 1, and the relative dielectric constant of the insulating medium ε_r is 3.6–4.5 [12], as shown in Figure 1. Under the applied voltage, the air gap will bear a higher voltage than the insulating pressboard, and the withstand voltage of air is much lower than that of the insulating paperboard, so the air gap will break down in advance. This is a typical partial discharge phenomenon caused by air gap defects. Based on the plasma fluid model, this paper will build a two-dimensional air gap model of oil-paper insulating paperboard to study this phenomenon [29,30].

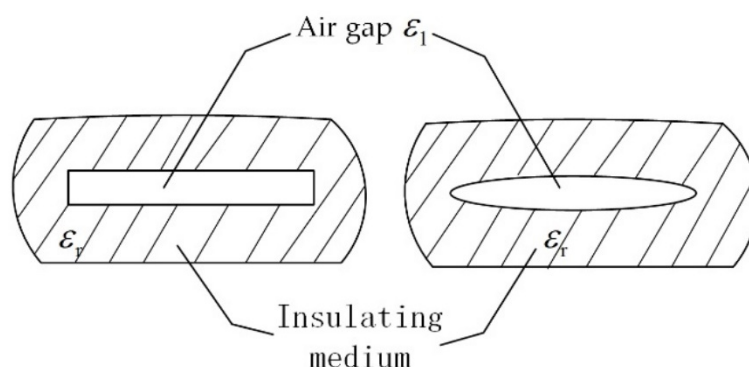


Figure 1. The model of air gap in an insulation board.

2.2. The Introduction of the Model Simulation

A two-dimensional axisymmetric model is built using COMSOL Multiphysics, as shown in Figure 2. The model consists of a uniform dielectric material epoxy resin with a width of 0.3 mm, a length of 2 mm and a relative dielectric constant $r = 3.6$, and a cylindrical cavity with a thickness of 0.1 mm and a length of 1 mm. The cavity is filled with atmospheric air at a temperature of 300 K.

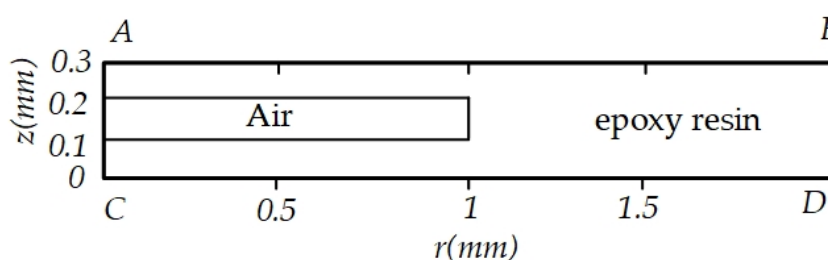


Figure 2. The model of simulation.

2.2.1. The Ratio of Combined Voltage

In order to build a better model, the AC–DC ratio of externally applied combined voltage used in this simulation refers to the AC–DC ratio used by the valve side winding of a converter transformer in an insulation withstand test. According to the test requirements of the Institute of Electrical and Electronics Engineers (IEEE) and the International Large Power Grid Conference (CIGRE), the insulation withstand test voltage at the valve side of a ± 800 kV converter transformer is jointly determined by DC component V_{DC} and AC component V_{AC} . Considering the loss of the smoothing reactor and rectifier circuit, the voltage of a single rectifier bridge in a converter transformer is

$$V_{dr} = 1.175 V_{ac}, \quad (1)$$

where V_{ac} is the power supply voltage of the rectifier bridge, and the AC component of the withstand test voltage at the valve side of the converter transformer is:

$$V_{AC} = V_{ac} / \sqrt{3}, \quad (2)$$

The DC component of withstand test voltage V_{DC} is:

$$V_{DC} = (p - 0.5) V_{dr}, \quad (3)$$

where p represents the number of rectifiers. There are four rectifiers in the ± 800 kV converter transformer. Replace $p = 1, 2, 3$, and 4 into Equation (3) successively. It can be seen that the ratio of AC effective voltage to DC average voltage in the withstand test voltage at the valve side of the transformer is 1:1, 1:3, 1:5, and 1:7, respectively.

In the simulation, the AC voltage component V_{AC} with frequency ($f = 50$ Hz) and the DC voltage component V_{DC} with different ratios ($V_{DC} + V_{AC} = 1.49$ kV) are applied to the upper surface AB of the simulation model, and the lower surface CD of the model is grounded. The total amplitude of the applied AC–DC combined voltage of the model has always been 1.49 kV, but the AC–DC component proportions of the composite voltage are 1:1, 1:3, 1:5, and 1:7, respectively.

2.2.2. Partial Discharge Numerical Simulation Model

Based on the work of previous researchers, the simulation model in this paper considers the main particles and chemical reactions in the air [28]. The main particles considered are: electrons, N_2^+ , N_4^+ , O_2^+ , O_4^+ , O^- , and O_2^- ions, N and O ground state atoms, N_2 , O_2 , and O_3 ground state molecules, O (1D) excited state atoms, N_2 (A) and N_2 (B) electron excited state nitrogen molecules, N_2 ($v = 1-4$) and O_2 ($v = 1-2$) vibrational excited state molecules, and O_2 (a), O_2 (b), and O_2 (c) electron excited state oxygen molecules [28,30]. Additionally, the chemical scheme is shown in the Appendix A (Tables A1 and A2). Note that the rate coefficients of electron-collision reactions $f(\bar{\epsilon})$ are precalculated by Bolsig + software with the cross-section data taken from, as well as the electron energy distribution function (EEDF). The relationship between $f(\bar{\epsilon})$ and EEDF is given by the following integral [31]:

$$f(\bar{\epsilon}) = \int_0^\infty \sqrt{\frac{2e}{m_e}} \epsilon \sigma_l F_{\bar{\epsilon}}(\epsilon) d\epsilon \quad (4)$$

here, e is the elementary charge, ϵ is the electron energy, σ_l is the collision cross-section for reaction l , and $F_{\bar{\epsilon}}(\epsilon)$ is EEDF. It is worth noting that $f(\bar{\epsilon})$ is the function of the mean energy [31].

The electron migration and other relevant particle parameters of the model are analyzed by the Boltzmann equation, and electron energy density is obtained by solving the continuity equations through the drift-diffusion approximation:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = S_e, \quad (5)$$

$$\frac{\partial n_\epsilon}{\partial t} + \nabla \cdot \Gamma_\epsilon = S_\epsilon - E \cdot \Gamma_e, \quad (6)$$

$$\Gamma_e = -\mu_e n_e E - D_e \nabla \cdot n_e, \quad (7)$$

$$\Gamma_\epsilon = -\frac{5}{3} \mu_e n_e E - \frac{5}{3} D_e \nabla \cdot n_e, \quad (8)$$

where n_e and n_ϵ are the electron number density and electron energy in the simulation, respectively, and the initial values are set as 2×10^6 [m³] and 3 [eV], respectively. Γ_e and Γ_ϵ represent electron flux and electron energy flux, respectively. The source term S_e describes the change in n_e due to the chemical reaction, and the electron energy source

term S_e represents the energy change caused by inelastic collision. E represents the electric field strength, and $E \cdot \Gamma_e$ stands for Joule heat. μ_e represents electron mobility [31,32].

The electron diffusion coefficient D_e is obtained by using Einstein's relation

$$D_e = \mu_e T_e \quad (9)$$

where the electron temperature T_e is calculated by:

$$T_e = \frac{2}{3} \bar{\varepsilon} = \frac{2n_e}{3n_e} \quad (10)$$

where $\bar{\varepsilon}$ is the mean electron energy.

The transport process of different heavy particles is solved by the multicomponent diffusion equation:

$$\rho \frac{\partial \omega_k}{\partial t} = \nabla \cdot j_e + S_k, \quad (11)$$

where ρ represents the density of the mixture, ω_k is the mass fraction, S_k is the source term, and j_k is the flux vector.

The Poisson equation is used to describe the potential distribution in the air gap:

$$\nabla \cdot (\varepsilon_0 \varepsilon_r \nabla \varphi) = \rho_v, \quad (12)$$

where ε_0 is the vacuum dielectric constant, φ is the potential, and ρ_v is the space charge density [33].

In partial discharge, the particles in the air gap will interact with the air gap surface and accumulate on the air gap surface. The following equation is characterizing the interaction between particles and air gap wall:

$$\mathbf{n} \cdot \Gamma_e = \frac{1}{2} v_{e,th} n_e - \alpha_s n_e \mu_e E \cdot \mathbf{n} - \sum_i \gamma_i (\Gamma_i \cdot \mathbf{n}), \quad (13)$$

$$\mathbf{n} \cdot \Gamma_\varepsilon = \frac{5}{6} v_{e,th} n_\varepsilon - \alpha_s n_\varepsilon \mu_\varepsilon E \cdot \mathbf{n} - \sum_i \gamma_i \varepsilon_i (\Gamma_i \cdot \mathbf{n}), \quad (14)$$

$$v_{e,th} = \sqrt{\frac{8T_e}{\pi m_e}}, \quad (15)$$

The electron flux and electron energy density on the wall can be obtained by the above formula [34]. The boundary condition of surface charge density ρ_s in the simulation can be solved according to the following formula:

$$\frac{\partial \rho_s}{\partial t} = \mathbf{n} \cdot J_e + \mathbf{n} \cdot J_i, \quad (16)$$

$$\rho_s = \mathbf{n} \cdot (D_1 - D_2), \quad (17)$$

where J_e and J_i are the electron current density and ion current density, respectively, and D_1 and D_2 are the potential displacement vector of the dielectric layer boundary in the air gap, respectively.

In order to ensure the conservation of total molar mass of the simulation model, the boundary conditions of heavy particles are:

$$\mathbf{n} \cdot j'_k = M_k R_{surf,k} + \alpha_s M_k c_k \mu_{k,m} z_k E \cdot \mathbf{n} \quad (18)$$

where j'_k , M_k , $R_{surf,k}$, and c_k represent the flux, molar mass, surface reaction rate, and mass fraction of heavy particles, respectively [32–40].

In this paper, the simulation research will be carried out based on the above model. The previous research of our research group shows that in the partial discharge with a similar

geometric size, the photoionization reaction will not affect the discharge morphology of partial discharge. Therefore, photoionization is not considered in this paper [27,28].

3. Results

In the simulation of this paper, the length and width of the air gap and the amplitude of the applied voltage of the model are fixed. We compared the discharge evolution process by adjusting the AC–DC ratio in the combined voltage. Previously, Mai Hong et al. conducted a large number of experiments on oil-paper air gap partial discharge under combined voltage with different AC–DC ratios and found that there is polarity effect in partial discharge [38]. When the DC component of the combined voltage increases, the discharge mainly occurs in the half cycle of the same polarity of the AC component and DC component. When the AC–DC ratio exceeds 1:1, the role of the DC component becomes more and more prominent until there is almost no discharge in another half cycle with opposite AC and DC polarity [41,42].

In order to observe the polarity effect of partial discharge under combined voltage, the normalized periodic electron density spatial distribution diagram under different AC–DC ratios of combined voltage is obtained by simulation, and the axial electron distribution of the air gap in a cycle can be known by Figure 3. In Figure 3, the R axis of this figure is the axial width of the air gap of the model, and the Z axis represents the timeline of the tenth discharge cycle of the simulation. In this simulation, we run ten discharge periods. Figure 3 is the normalized distribution of electron density in the tenth period. Additionally, 0.19 in Figure 3 represents the half period of the tenth period, which is the AC voltage component from the positive half period to the negative half period.

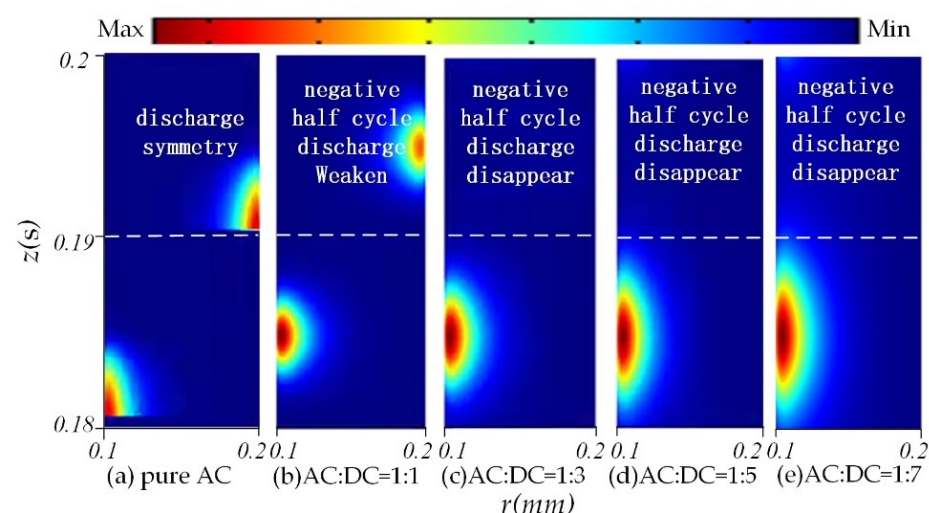


Figure 3. Normalized periodic electron density under different ratios of combined voltage. (a) pure AC, (b) AC:DC = 1:1; (c) AC:DC = 1:3; (d) AC:DC = 1:5; (e) AC:DC = 1:7.

As can be seen from Figure 3a, when the applied voltage is pure AC voltage, the discharge will occur in the positive and negative half cycle, the electron density distribution area is similar, and the magnitude of electron density is of the same order. When the AC/DC ratio of the applied voltage is 1:1, it can be seen that although the discharge occurs in both positive and negative half cycles, it is obvious that the electron density distribution area in the positive half cycle is larger and the order of magnitude of electron density is higher, as shown in Figure 3b. Once the ratio of AC–DC exceeds 1:1, it can be seen from Figure 3c–e that the discharge is concentrated in the positive half cycle, and the negative half cycle discharge is almost invisible. Comparing Figure 3c–e, it is found that when the DC component in the combined voltage increases, the electron aggregation region in the positive half cycle gradually increases, centered on the position of 1/4 cycle (0.185 s).

Combined with the simulation results and the experimental results of previous scholars, it can be seen that when the DC component in the applied combined voltage is significantly greater than the AC component, the electric field vector direction in the air gap is consistent with the polarity of the DC voltage component and will not change with the polarity of the AC component. At this time, the strong discharge in the air gap is concentrated in the positive half cycle, in which the AC component and DC component have the same polarity. Moreover, when the proportion of the DC component in the combined voltage is large, even if the polarity of the AC voltage changes, the DC voltage applied to the upper plate can still attract a large amount of electron aggregation. Therefore, the electron aggregation region in Figure 3c–e expands with an increase in the DC component. The simulation results are consistent with the experimental results of Mai Hong [41]; the partial discharge under the combined voltage does have a polarity effect.

From the above simulation results, it is easy to see that the partial discharge phenomenon under the combined voltage with an AC–DC ratio of 1:1 in Figure 3b is similar to that under pure AC voltage in Figure 3a. The partial discharge phenomenon under the combined voltage with an AC–DC ratio of 1:3, 1:5, and 1:7 is quite different from that under the pure AC voltage. Therefore, in order to better analyze the role of the DC component in the combined voltage, our work focuses on analyzing the results from a simulation, which is under the AC–DC voltage ratios of 1:3, 1:5, and 1:7 [43–46].

4. Analysis

In order to further study the influential mechanism of the DC component in a combined voltage acting on the partial discharge and verify the conjecture of scholars about the action mechanism of the DC voltage component, we have drawn Figure 4 to compare the effect of the DC voltage component in the combined voltage. Figure 4 shows the change in charge density on the upper surface in the model at the peak time of the fifth and tenth discharge in the air gap under 1:3, 1:5, and 1:7 combined voltages. When the discharge reaches the fifth and tenth times, the charge distribution in the air gap is almost stable, which can help us better qualitatively analyze the simulation results.

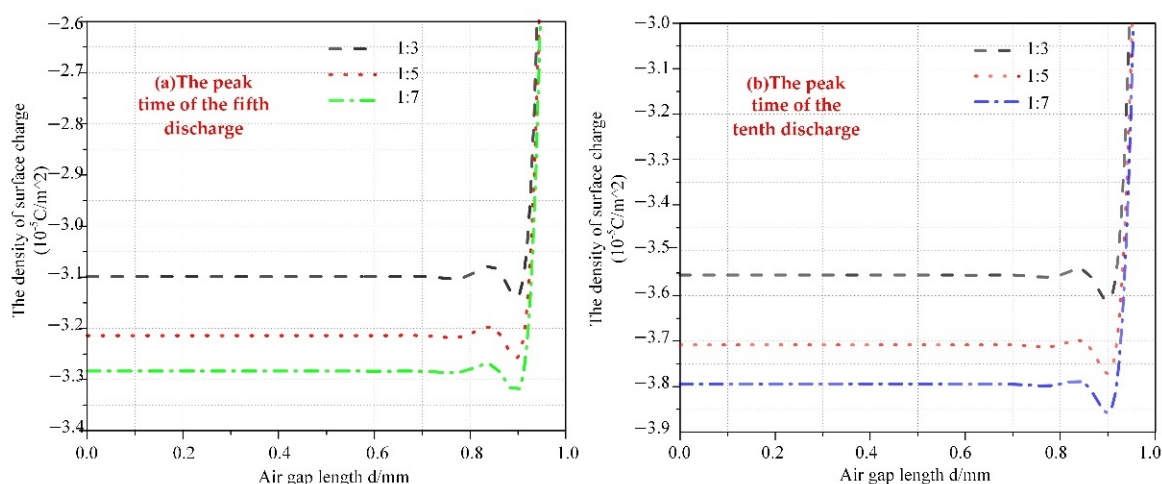


Figure 4. The density of surface charge at the fifth and the tenth discharge peak. (a) The peak time of the fifth discharge. (b) The peak time of the tenth discharge.

Figure 4 shows the radial surface charge distribution inside the air gap. From the figure, it can be found that the surface charge density is a straight line at the left and middle of the air gap without much change. At the right edge of the air gap, the surface charge increases suddenly. In order to further study the reason for the sudden increase in charge here, Figure 5 shows the electron density evolution diagram of the tenth discharge cycle under the combined voltage with an AC–DC ratio of 1:3. The change in electron density

under combined voltage with ratios of 1:5 and 1:7 is similar to that of 1:3, so 1:5 and 1:7 are not listed here.

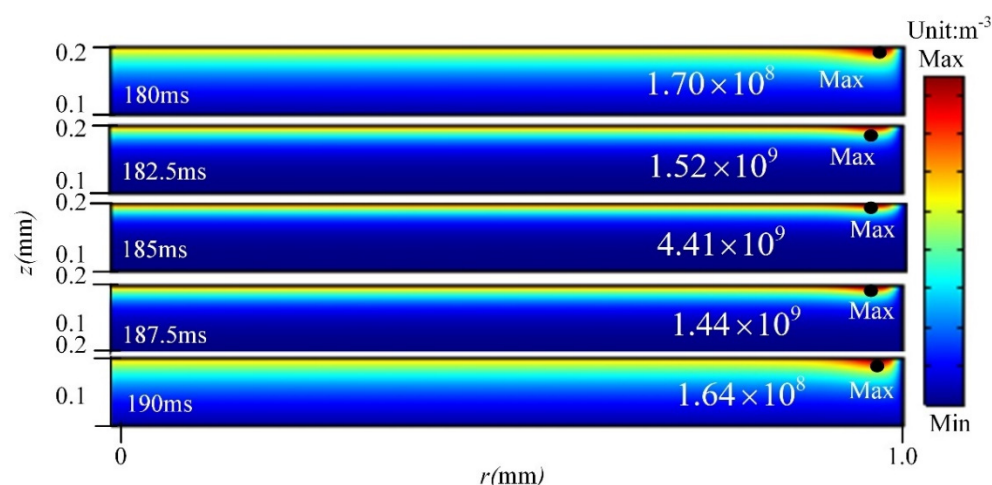


Figure 5. Evolution of spatial distribution of electron density in the 10th discharge air gap under composite voltage of 1:3.

As can be seen from Figure 5, the maximum electron density appears on the right side of the air gap. It can be seen that the strong partial discharge in the air gap occurs here. As can be seen from Figure 6, the electric field distortion occurs at the edge of the air gap. Due to the Townsend ionization coefficient, α in the collision ionization equation is positively correlated with the electric field intensity, so the strong partial discharge first appears in the middle. With the development of discharge, more and more charges are accumulated in the middle, and a large number of accumulated space charges inhibits the internal discharge. In the tenth discharge cycle of Figure 5, the partial strong discharge has moved to the right of the air gap. The surface charge density on the right side of Figure 4 decreases sharply after a sudden increase because it is close to the insulating material wall.

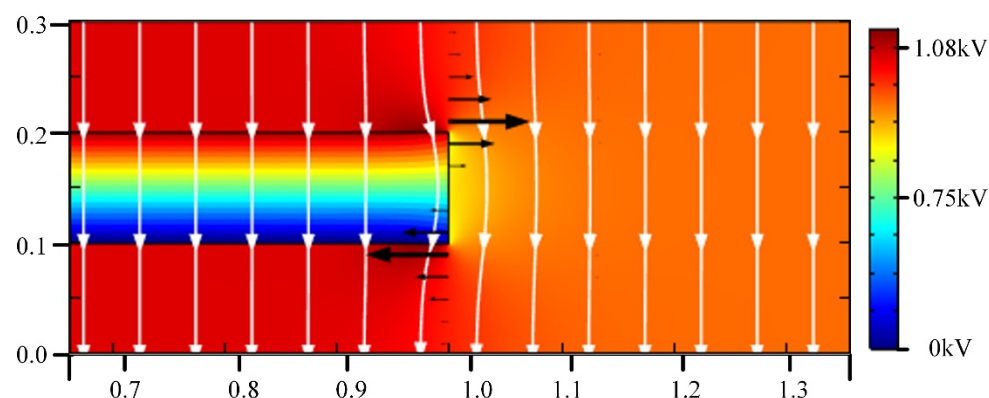


Figure 6. Distribution of electric field and potential at peak discharge moment.

It can be seen from Figure 4 that when the DC component in the combined voltage increases, the surface charge density increases. In addition, the surface charge density at the tenth discharge peak is higher than that at the fifth discharge peak. Thus, we predicted that with the development of discharge, the surface charge will accumulate.

In order to further analyze the effect of the DC voltage component acting on the space charge in the air gap, Figure 7 shows the spatial distribution of positive ions in the air gap under each AC–DC combined voltage ratio. As shown in Figure 7, it can be found that under the combined voltage with an AC–DC ratio of 1:1, the spatial distribution of positive ions is mainly concentrated in the strong discharge area on the right side of the

air gap, and the distribution of positive ions in other areas in the air gap is relatively thin. Comparing the spatial distribution of positive ions under the combined voltage with an AC–DC ratio of 1:3, 1:5, and 1:7, it is found that the distribution of positive ions is more dispersed, and the concentration is more uniform with an increase in the DC component. It can be seen from Figure 3 that different from the amplitude of the AC voltage changing with time, when the DC voltage component increases, the air gap is continuously affected by the electric field with the same polarity as the DC voltage throughout the discharge cycle. Therefore, under the effect of the fixed electric field, the distribution of space charge will be more uniform and dispersed, resulting in the expansion of the discharge area, but the discharge intensity is obviously weakened.

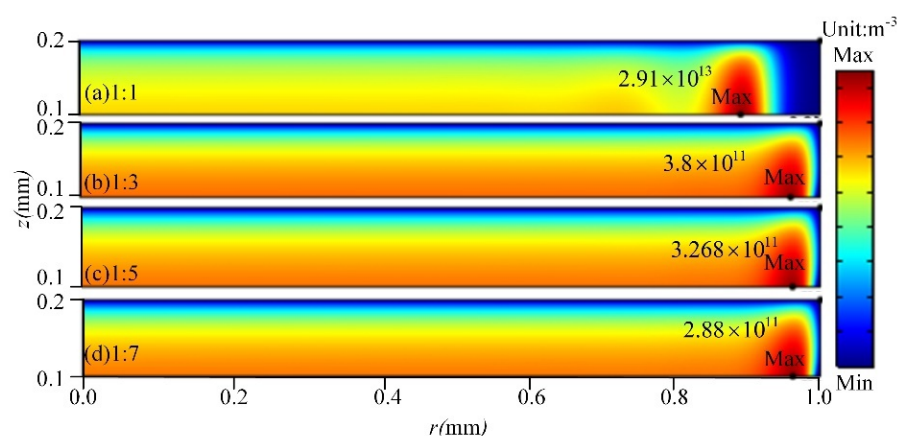


Figure 7. The spatial distribution of positive ions.

According to the analysis of Figures 4 and 7, when the DC voltage component increases, the surface charge density in the air gap increases and the space charge distribution becomes more dispersed. In conclusion, the simulation results in this paper are consistent with the previous analysis of scholars that an increase in the DC voltage component will cause an increase in surface charge and space charge [17–21].

Comparing the spatial distribution of positive ions under each combined voltage ratio in Figure 7, we found that the density of positive ions decreases with an increase in the DC voltage component. We believed when the DC voltage component increases, the surface charge and space charge in the air gap become more active, resulting in a large number of charges gathering on the surfaces of the upper and lower plates. Finally, an electric field with opposite polarity to the applied external DC voltage component is generated in the air gap, which weakens the effect of the external combined voltage and inhibits the development of strong discharge in the air gap. To verify this conjecture, we drew the potential distribution at the peak time of the fifth and tenth discharge under each combined voltage ratio, as shown in Figure 8.

Figure 8 shows the surface potential inside the air gap under 1:3, 1:5, and 1:7 combined voltages. It can be seen that the surface potential of the air gap gradually decreases with an increase in the DC voltage component in the composite voltage. This phenomenon will weaken the strong discharge phenomenon in the air gap, resulting in a decrease in positive ion density and electron density in the air gap. Comparing the two figures (a) and (b) of Figure 8, it is found that the potential decreases gradually with the development of discharge. It can be seen from the above that with the development of discharge, the upper and lower surface charges in the air gap will accumulate. Thus, a larger reverse electric field is generated in the air gap, which reduces the potential in the air gap.

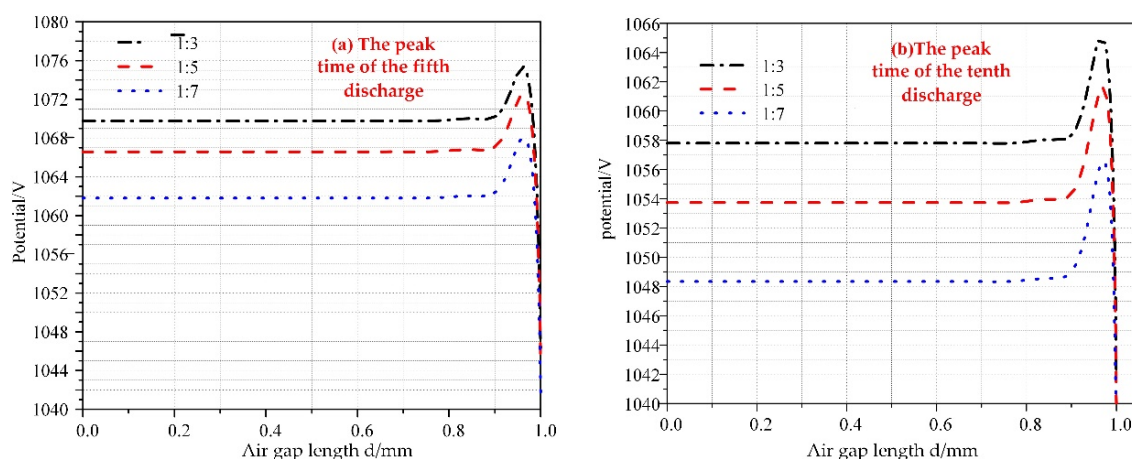


Figure 8. The potential at the fifth and the tenth discharge peak. (a) The peak time of the fifth discharge. (b) The peak time of the tenth discharge.

The simulation results in this paper qualitatively conform to the experimental phenomena of Li, Qi, and Sha and clarify the evolution process of partial discharge in air gap under combined voltage from a physical perspective.

5. Conclusions

Based on the plasma fluid model, the partial discharge characteristics and evolution mechanism of an oil-paper insulation structure of a converter transformer under AC–DC combined voltage are studied in this paper.

The numerical simulation shows that with an increase in the DC component in the combined voltage, the discharge area in the air gap expands, but the discharge intensity decreases obviously. This is because when the DC voltage component is large, the air gap is continuously affected by the electric field of the same polarity as the DC voltage, which makes the particles in the air gap more active and the space charge distribution more dispersed. With an increase in the DC voltage component in the combined voltage, the surface charge density in the air gap increases accordingly, and a large number of charges accumulate on the upper and lower surfaces of the air gap. Thus, an electric field opposite to the polarity of the DC component in the combined voltage is generated, which weakens the applied combined voltage and reduces the potential in the air gap.

The simulation results in this paper are qualitatively consistent with the experiment and simulation results of previous researchers. An increase in the DC component in the combined voltage can effectively reduce the strong discharge phenomenon in the air gap, so as to reduce the incidence of partial discharge. In this paper, the mechanism of partial discharge under AC/DC combined voltage is studied by simulation, which not only defines the evolution process of partial discharge in oil-paper insulating paperboard under combined voltage from the perspective of micro particles, but also provides a new idea and direction for reducing the occurrence of partial discharge in practical engineering.

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Appendix A

Table A1. Gas-phase reactions considered in the model.

Reaction No.	Reaction Equation	Rate Constant	Threshold (eV)	Ref.
1	$e + N_2 \Rightarrow e + N_2$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[46]
2	$e + N_2 \Rightarrow e + N_2 \text{ (} v = 1\text{--}4\text{)}$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	0.2889, 0.8559, 1.1342	[46]
3	$e + N_2 \Rightarrow e + N_2(A)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	6.1688	[46]
4	$e + N_2 \Rightarrow e + N_2(B)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	11.03	[46]
5	$e + N_2 \Rightarrow 2e + N_2^+$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	15.6	[46]
6	$e + O_2 \Rightarrow e + O_2$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[46]
7	$e + O_2 \Rightarrow e + O_2 \text{ (} v = 1\text{--}2\text{)}$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	0.57, 0.75	[46]
8	$e + O_2 \Rightarrow e + O_2(A)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	0.977	[46]
9	$e + O_2(A) \Rightarrow e + O_2$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	−0.977	[46]
10	$e + O_2 \Rightarrow e + O_2(B)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	1.627	[46]
11	$e + O_2(B) \Rightarrow e + O_2$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	−1.627	[46]
12	$e + O_2 \Rightarrow e + O_2(C)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	4.5	[46]
13	$e + O_2 \Rightarrow O + O^-$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[46]
14	$e + O_2 \Rightarrow O_2^-$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[46]
15	$e + O_2 \Rightarrow e + O + O$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	5.58	[46]
16	$e + O_2 \Rightarrow e + O + O(^1D)$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	8.4	[46]
17	$e + O_2 \Rightarrow 2e + O_2^+$	$f(\bar{\epsilon}) \text{ (m}^3 \text{ s}^{-1}\text{)}$	12.1	[46]
18	$e + N_2 \Rightarrow e + N + N$	$1 \times 10^{-14} \times T_e^{-0.5} \exp(-16/T_e) \text{ (m}^3 \text{ s}^{-1}\text{)}$	9.757	[24]
19	$e + N_2^+ \Rightarrow N + N$	$4.8 \times 10^{-13} (T_e/0.026)^{-0.5} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[25]
20	$e + N_4^+ \Rightarrow 2N_2$	$2 \times 10^{-12} (T_e/0.026)^{-0.5} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[25]
21	$e + O_2^+ \Rightarrow 2O$	$1.2 \times 10^{-14} T_e^{-0.7} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
22	$e + 2O_2 \Rightarrow O_2 + O_2^-$	$5.17 \times 10^{-43} T_e^{-1} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[24]
23	$e + O_2^+ \Rightarrow O_2$	$4 \times 10^{-18} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
24	$e + O_4^+ \Rightarrow 2O_2$	$2.25 \times 10^{-13} T_e^{-0.5} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
25	$N_2^+ + 2N_2 \Rightarrow N_4^+ + N_2$	$1.9 \times 10^{-41} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[25]
26	$N_4^+ + N_2 \Rightarrow N_2^+ + 2N_2$	$2.5 \times 10^{-21} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[25]
27	$O^- + O_2^+ \Rightarrow O + O_2$	$1 \times 10^{-13} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[47]
28	$O_2^- + O_2^+ \Rightarrow 2O_2$	$4.2 \times 10^{-13} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[47]
29	$O_2^- + O_2^+ + O_2 \Rightarrow 3O_2$	$2 \times 10^{-37} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[47]
30	$O_2^- + O_2^+ + N_2 \Rightarrow 2O_2 + N_2$	$2 \times 10^{-37} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[47]
31	$O_2^- + O_4^+ + O_2 \Rightarrow 4O_2$	$2 \times 10^{-37} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
32	$N_2^+ + N_2 + O_2 \Rightarrow N_4^+ + O_2$	$5 \times 10^{-41} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
33	$N_4^+ + O_2 \Rightarrow O_2^+ + 2N_2$	$2.5 \times 10^{-16} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[48]
34	$O_2^+ + 2O_2 \Rightarrow O_4^+ + O_2$	$2.4 \times 10^{-42} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
35	$O_2^- + O_4^+ + N_2 \Rightarrow 3O_2 + N_2$	$2 \times 10^{-37} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
36	$O_2 + N + N \Rightarrow O_2 + N_2$	$3.9 \times 10^{-45} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[25]
37	$O + O + N \Rightarrow O_2 + N$	$3.2 \times 10^{-45} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[25]
38	$O + O_2 + N_2 \Rightarrow O_3 + N_2$	$6.2 \times 10^{-46} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
39	$O + O_2 + O_2 \Rightarrow O_3 + O_2$	$6.9 \times 10^{-46} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[48]
40	$O^- + O_2^+ + N_2 \Rightarrow O_3 + N_2$	$2 \times 10^{-37} \text{ (m}^6 \text{ s}^{-1}\text{)}$	/	[35]
41	$O + O_4^+ \Rightarrow O_3 + O_2^+$	$3 \times 10^{-16} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[48]
42	$O + O_3 \Rightarrow O_2 + O_2$	$8 \times 10^{-18} \exp(-2060/300) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
43	$O^- + O_3 \Rightarrow O_2 + O_2 + e$	$3 \times 10^{-16} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
44	$N_2^+ + O_3 \Rightarrow N_2 + O + O_2^+$	$1 \times 10^{-16} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
45	$e + O_3 \Rightarrow O_2 + O + e$	$1.78 \times 10^{-12} (3T_e/2)^{-0.614} \exp(-23/3T_e) \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
46	$e + O_3 \Rightarrow O + O_2^-$	$1 \times 10^{-15} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]
47	$e + O_3 \Rightarrow O_2 + O^-$	$1 \times 10^{-17} \text{ (m}^3 \text{ s}^{-1}\text{)}$	/	[24]

Table A2. Surface reactions considered in the model.

Number	Surface Reaction	Reaction Probability	γ_i	Initial Electron Mean Energy
S1	$N_2^+ + \text{Surface} \Rightarrow N_2$	1	6.5×10^{-4}	3
S2	$N_4^+ + \text{Surface} \Rightarrow 2N_2$	1	6.5×10^{-4}	3
S3	$2O^- + \text{Surface} \Rightarrow O_2$	1	0	0
S4	$O_2^- + \text{Surface} \Rightarrow O_2$	1	0	0
S5	$O_2^+ + \text{Surface} \Rightarrow O_2$	1	6.5×10^{-4}	3
S6	$O_4^+ + \text{Surface} \Rightarrow 2O_2$	1	6.5×10^{-4}	3

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