Application of Molecular Dynamics Study and Homo-Lumo Calculation on the Ionized Air for High Voltage Engineering

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Application of Molecular Dynamics Study and Homo-Lumo Calculation on the Ionized Air for High Voltage Engineering

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***Abstract*— Air is a gas insulation in high voltage engineering. Generally, the air content consisted of several gas elements like N_2, CO_2, CO, H_2, CO, and O_2. Sunlight can cause the air ionization, the air ionization can resulted because of the high electric fields and also the interaction between electrons from gas molecules. The air which ionized in the high voltage, leads to the event of isolation failure or better known as the failure process of Streamer and Townsend. The main purpose of this research was to get a better insight of air ionization process. Tools such as molecular dynamic and SCF calculation can be used to achieve this goal. For the CO_2 molecule, the best pose was selected at the time value of 1.000 s with the energy of 0.0502 kcal/mol,at temperature of 120.440 K and pressure of 1260386 barr. While the other gas, N_2 molecule, is seems to be stable under ionization process. Thus, for this molecule, the best pose was found at the time value of 1.000 s, energy of 0.0526 kcal/mol, with temperature of 205.949 K and pressure of 78539.601 barr. Based on the molecular dynamic results, O_2 molecule will be ionizes at time value of 1.000, energy of 0.430 kcal/mol, with temperature of 0.0104 K and pressure of 18498.320 barr. SCF calculation give the energy ionization potential value for N_2, CO_2, O_2, H_2, N_2 and O_2, CO_2 and O_2, CO_2 N_2 and O_2 of 9.38 eV, 11.81 eV, 9.38 eV, 11.99 eV, 9.38 eV, 9.38 eV, 9.38 eV, respectively. Based on this calculation, the molecule with lowest potential ionization energy can ionized easier. N_2, NO_2, N_2 gases and O_2, CO_2 and O_2, CO_2, N_2 and O_2 are ionized easier than gas CO_2 and H_2 .**

Keywords— Molecular dynamic, ionized air, gases insulation, ionization energy, Homo-lumo, high voltage.

I. Introduction

Generally, high voltage engineering is a part of electrical engineering which is included the study and also the application of electrical phenomena of occurring in various mediums at high voltages. High voltage engineering is also included the knowledge of insulation failure of solid, liquid and gas. Air consists of elements like N_2, CO_2, CO, H_2, CO, and O_2. Computational approach can be used to study the air failure in the high voltage which can be utilized to generate ozone from the ionization process of the oxygen atoms. In this research, we combined molecular dynamic simulation (MD) and homo-lumo calculation to study the ionization process of these gas elements.

This research attempts to compare the temperature, time, pressure and ionization potential energy for each gases insulation. The data obtained is used to demonstrate the stability of each gas in the ionization process also it can be used to research the gas that is difficult to ionize.

II. Review

Molecular dynamic (MD) simulation can be defined as a procedure to obtain the system routes for the classical dynamics. The time average as a part of the properties of the system can also then be determined. MD creates the usage of fixed in the difference combination of algorithms: at the certain time, atoms force are measured and pooled with the recent position to produce a new position and also the velocities to generate new velocities in a very short time for each step ahead [1]. The performance of each atom is expected to be closely with the constant through this time step. Then, the predicted for the new atomic with new position, computed the updated of forces set and dynamic cycle goes on.

The computational approach can be used to know the properties of the assembly molecules during the structure and intereraction of microscopic between all the atoms, this called the conventional experiment. Furthermore, it can be used for the researchers to discover soething new. Currently, molecular dynamic simulation is a new procedure that can be applied for understanding about the atomic, interaction between the atom and also the molecular algorithm.

The simulation techniques can be classified into two main classes, they are, Molecular Dynamics (MD) and Monte Carlo (MC) [2]. MD was applied to run a mesoscale model like thermal shocks, that MD was able to elucidate accurately the process of non-equilibrium. In the MD simulation, the main essential factors is Planck constant [3, 4]. The Planck constant, *h*, is a physical constant that is the quantum of action, and can generally generated as $E = h \upsilon$, where E is energy, h is planck constant and υ is frequency. Base on this equation, for the ionization process MD were performance to see whether these three paramaters are important or not.

The ionization potential of a molecule can be approximated as the HOMO (highest occupied molecular orbital) and LUMO (lowest occupied molecular orbital). HOMO is the valence orbital that received the last valence electrons. The LUMO is the empty orbital just above the HOMO. A molecule consists of proton and electron. Molecule can make bonds with using the electrons together between them, and probably, the chemical bond was also can be perform by sharing two electrons by two atoms. Atoms can used together one electron to perform single bond, two electron to perform double bonds or three electrons to create triple bonds. For example for gas hydrogen, it is consisted of a nucleus (a *proton*) and an *electron*. It is possible to calculate the possiblity of finding electron at any point surrounding the nucleus for the hydrogen atom, unfortunately, it is not possible to determine where is exactly the electron.

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are the main important properties for an atom or molecule. Frontier orbital can be formed when the HOMO and LUMO are stayed together. HOMO can be found if an electron is putting in the outer of the orbital and LUMO can be found if there are no electron in the first orbital [5, 6]. There are some reasons to make the frontier orbitals become so significant, they are:

1. Method for calculating the ionization energy.
2. Koopman's Theory.

The HOMO involed in these methods, where the ionization enery is equal to the energy of the orbital from which the electron is ejected. This means that the ionization energy is equal to the HOMO energy.

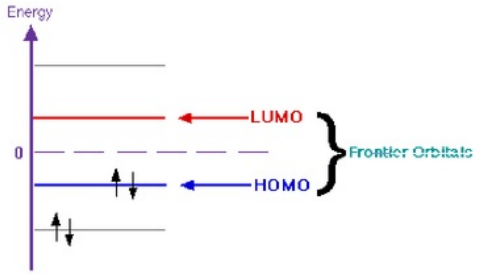

Fig.1 Diagram of HOMO and LUMO

III. Material Method

Molecular Dynamics (MD) simulations were conducted to check the stability of the gas elements N_2, O_2, CO, CO_2, H_2, N_2 and O_2, CO_2 and O_2, CO_2 N_2 and O_2. Molecular dynamics simulation consists of statistical and also some equations. MD is very important to solve the atomic problem, for this, the MD simulation have to collaboorate with the force filed. Force field is the properties and vibration frequencies, there are some classification of this force field, such as AMBER17, AMBER18, CHARMM19 and OPLS20 are geared more to larger molecules in condensed phase [7, 8]. In this research, the preliminary studieds of molecular dynamic simulation was performed using NAMD (Nanoscale Molecular Dynamics program v 2.9). CHARMM19 (Chemistry at Harvard Macromolecular Mechanics) was used as the best force field, NPA was then used as algorithm and NVT was used as ensemble parameter [9].

All the structure of the gas elements were sketched using ChemDraw ultra followed with minimization energy using MOPAC. Before running the homo-lumo calculation, the following paramater have to be prepared such as AM1 was selected as the basis set, MOPAC was selected as an engine, and singlet/closed was selected as the multiplicity. Furthermore after the parameter was set up, the homo-lumo calculation can start to run and it is presented in Fig.1.

IV. Result and Discussion

Molecules or other groups of atoms are described via single particles, are an attractive alternative to all atoms. MD and homo-lumo calculation to study shock induced process because they involve spatial and temporal scales that go beyond those attainable at the atomistic level. The ionization process of gases such as N_2, O_2, CO, CO_2, H_2, N_2 and O_2, CO_2 and O_2, CO_2 N_2 and O_2 can also measure using molecular dynamic simulation. From this MD simulation, we will know time, pressure, volume and temperature for the ionization process. Homo-lumo calculation provides the energy of ionization potential for these gas elements.

A. Molecule N_2

The gas N_2 is look like little bit stable for the ionization process. Based on MD simulation, at the best pose selected with the following results; the time value of 1.000 s, energy of 0.0526 kcal/mol, with temperature of 205.949K and pressure of 78,539.601 bar were observed [10]. The ionization process of N_2 molecule is depicted in Fig. 2.

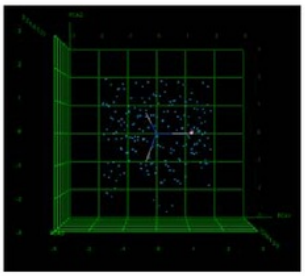

Fig.2 The ionization process of gas N_2

B. CO_2 Moleule

The best poses of MD for CO_2 gas reported as the time value of 1.000 s, energy of 0.0502 kcal/mol, at temperature of 120.440 K and pressure of 1,260,386 bar. In addition, CO_2 molecule seems to be able to ionize since it shown the energy of 0.0502 at the lowest time (1.000 s) [10]. Based on homo-lumo calculation, CO_2 molecule has the energy ionization potential of 11.81eV. The ionization process of CO_2 molecule is presented in Fig. 3

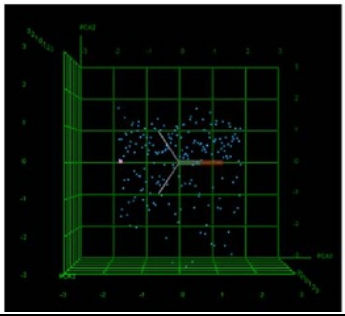

Fig.3 The ionization process of gas CO_2

C. O_2 Molecule

Molecular dynamic simulation was also performed for the O_2 gas. Likewise, from the molecular dynamic simulation O_2 gas shown that this gas is able to ionize at time value of 1.000, 0.430 kcal/mol energy, at temperature of 0.0104 K and pressure of 18,498.320 bar. The ionization process of O_2 molecule is depicted in Fig. 4.

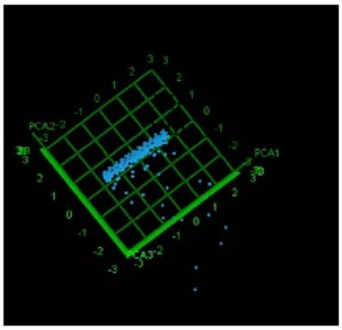

Fig.4 The ionization process of gas O_2

Homo-lumo calculation was also performed to this gas and it come out with the energy ionization potential of 9.38 eV. It seems like gas N_2 that gas O_2 is also easier to ionize.

D. H_2 Molecule

Hydrogen gas is a part of the gas elements. The molecular dynamic simulation was performed for this gas as well. It shown that this gas will be ionize on time value of 1.000, energy of 0.630 kcal/mol, with temperature of 150 K and pressure of 14,698.320 bar. Homo-lumo calculation was performed with the energy ionization potential of 11.99 eV. The ionization process of H_2 is presented in Fig. 5.

E. N_2 and O_2 Molecules

MD simulation was also performed to the mixture of N_2 and O_2 gases. It was observed that the mixture will be ionized at 1.000 s, 0.0026 kcal/mol energy, with temperature of 205.949K and pressure of 7,839.601 bar. Base on homo-lumo calculation, this mixture gas was observed the energy ionization potential of 9.38 eV. It indicated that this gas was able to ionize and also have high potential to break down the gas insulation at the certain high voltage level. the ionization process of gas N_2 and O_2 is shown in Fig. 6.

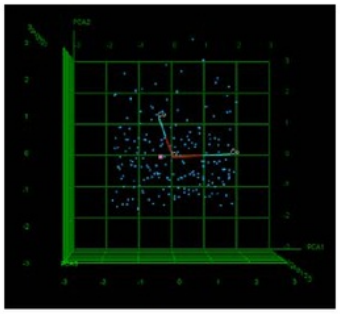

Fig.5 The ionization process of gas H_2

the ionization process of gas N_2 and O_2 is shown in Fig. 6.

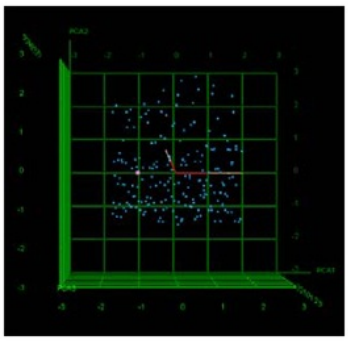

Fig.6 the ionization of gas N_2 and O_2

F. CO_2 and O_2 Molecules

Similar to the previous gas, the mixture of CO_2 and O_2 gas, also run using MD simulation and homo-lumo calculation. Based on MD simulation and homo-lumo calculation, this gas is seems to be able to ionize well and high potency to change the insulation and become conductively flow current in the gas insulation under the high voltage stress. From MD simulation, this gas has time of 1.000 s, energy of 0.0186 kcal/mol, at temperature of 1,078.949K and pressure of 608.839 bar. Base on homo-lumo calculation, this mixture was found to have the energy ionization potential of 9.38 eV. The ionization process of this gas is depicted in Fig. 7.

G. N_2, O_2 and CO_2 Molecules

The best poses of MD simulation for gas mixture of N_2, O_2 and CO_2 gas suggested that, this gas has time of 1.000 s, energy of 0.0895 kcal/mol, with temperature of 4,978.89K and pressure of 403.679 bar. Homo-lumo calculation, this gas

mixture was observed the energy ionization potential of 9.38 eV. Based on this calculation, the lowest energy ionization potential indicated that this gas mixture seems to be easily ionized. For high voltage, it is indicated that this gas easy to failure under high voltage stress. The ionization process of N_2, O_2 and CO_2 gas is depicted in Fig. 8.

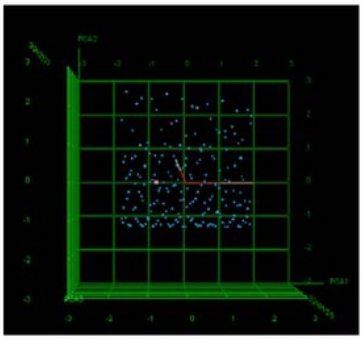

Fig.7 The ionization process of molecule CO_2 and O_2

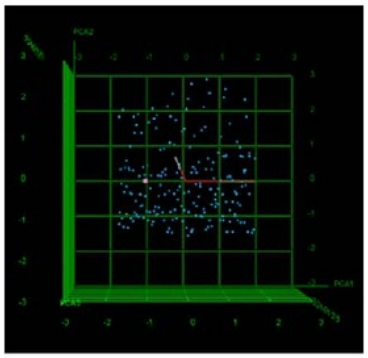

Fig. 8 The ionization process of gas N_2, O_2, CO_2

V CONCLUSION

There are several conclusions that can be concluded base on this research, they are:

1. Molecular dynamic simulation and homo-lumo calculation can be used to study the ionization process of gas in the high voltage insulation.
2. The lowest of the energy ionization potential indicated that the ionization process is easy and it is indicated that they have high potential to break down the gas insulation at the certain high voltage level.
3. N_2, NO_2, N_2 and O_2, CO_2 N_2 and O_2 gases are easier to ionized compare to CO_2 and H_2 gas.

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