IEEE Access
Multidisciplinary ⋮ Rapid Review ⋮ Open Access Journal

Received February 23, 2021, accepted March 3, 2021, date of publication March 10, 2021, date of current version April 8, 2021.

Digital Object Identifier 10.1109/ACCESS.2021.3065071

Simulation and Experiment of SF_6/N_2 Mixed Gas Distribution in High Vertical Drop GIL

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This work was supported in part by the Fundamental Research Funds for the Central Universities under Grant 2018JBM071.

ABSTRACT Dielectric breakdown of a vertical Gas insulated transmission line (GIL) caused by demixing of the mixture of SF_6/N_2 is studied by both theoretical simulation and the experimental measure. The mechanism and the threshhold of the demixing is addressed quantitatively. The potential risk of the segregation of the molecules by forming dimer or trimer under the high voltage is excluded by the quantum mechanics simulation in microscopic scale and the molecular simulation in mesoscopic scale. In macroscopic scale, the distribution of the mixture depending on the length of the tube is computed by the statistical physics quantitatively.

INDEX TERMS Experiment, separation of gas blend, SF_6/N_2 mixture, simulation.

I. INTRODUCTION

Gas insulated transmission line (GIL) is a kind of electric energy transmission equipment with metal shell, enclosed conductive rod, insulation gas and coaxial arrangement of shell [1], [2]. It has the characteristics of large transmission current, high transmission power, small volume and small floor area. It has significant advantages in high transmission capability and low energy loss [2]–[5]. Sulfur hexafluoride (SF_6) gas has good electrical and chemical insulating properties as well as heat transfer properties. For these reasons, SF6 gas has been used as insulating gas in GIL. The molecule has strong electronegativity. By combining with electrons to form negative ions, it prevents the occurrence of the electronic avalanche process. Therefore, it has high insulation properties and is suitable for use as insulation and arc extinguishing media of circuit breakers. However, SF_6 gas has a strong greenhouse effect (the global warming coefficient GWP is 23800) and has great impact on the environment. It is listed internationally as a restricted greenhouse gas. In 2001, Siemens developed the second-generation GIL [1], [6]–[8], using SF_6/N_2 mixed gas with SF_6 volume content of about 20%, and successfully piloted it in some countries [9]–[11]. In recent years, the State Grid Corporation of China has developed a 1100 kV SF_6/N_2 mixed gas GIL prototype. Compared with pure SF6 gas GIL, SF_6/N_2 mixed gas GIL greatly reduces the consumption of SF_6 gas, which not only has a significant environmental protection effect, but also reduces the cost by more than 50%.

Under the action of gravity, SF_6 gas and N_2 gas stratification may occur in the pipeline due to the large difference in the specific gravity of the two molecules. Especially at the large-scale vertical height, this effect can increase with the increase of spatial scale, which may cause a huge change in the relative ratio of SF_6/N_2 in the upper and lower layers of the insulated pipe [4]. As a result, under the low temperature, this great insulation properties is a hard problem should be concerned during the power gird design. The stratification can also cause insulation performance reduction, and even the gas breakdown. This difficulty problem has long plagued the high-voltage transmission design and application departments. Part of my country's hydropower and nuclear power plant projects have begun to use GIL as the way of power entry and exit, such as the 800 kV GIL project of Laxiwa Hydropower Station [5]. The engineering technology is difficult. The height difference of the shaft is more than 200 meters. Two GILs are used to transport electric energy from underground caverns to ground outlet stations, and then connect to overhead lines and merge into the grid. Starting from the polarization mechanism of micro-molecules, through multi-scale theoretical research, it is an important scientific problem to demonstrate the physical and chemical mechanism of insulating mixed gas stratification at the

The associate editor coordinating the review of this manuscript and approving it for publication was Fabrizio Messina.

principle level, and to explore the height limit of stratification on the macro-scale.

So far, the studies have concentrated on the insulation characteristics and discharge characteristics of SF_6/N_2 mixed gas [12]–[14]. The studies focusing on the physical and chemical properties of SF_6/N_2 mixed gas, especially the statement of SF_6/N_2 mixed gas in high vertical drop GIL gas chamber distribution were rarely reported. Yuchang *et al.* [15], Qi and Yuchang [16] used the gas equation of state to calculate the change of the SF_6/N_2 mixed gas ratio with height, and set up a simple experimental device.

In this paper, quantum mechanics is used to accurately calculate the interaction force between molecules of SF_6/N_2 mixed gas at the microscopic scale. Aiming at the polarization of molecules under power transmission conditions, a model of the interaction between molecules under the real working conditions of the GIL pipeline is established. The statistical behavior of SF_6/N_2 mixed gas in the GIL pipeline is simulated by molecular dynamics (MD). At the same time, an SF_6/N_2 mixed gas experimental platform with a height of 30 meters was built to detect the ratio of SF_6/N_2 mixed gas at different heights and provide theoretical and experimental data for the distribution of SF_6/N_2 mixed gas in the high vertical gas chamber, which have certain research value.

II. SIMULATION METHOD AND EXPERIMENTAL PLATFORM

A. SIMULATION METHOD

In this paper, a multi-scale simulation method is used to study the mixing and separation of SF_6/N_2 mixed gas in the gravitational field. On the microscopic electronic structure scale, the interaction between molecules in the SF_6/N_2 mixed gas is accurately calculated through quantum mechanics. For the polarization of molecules under power transmission conditions, we establish the interaction model between molecules under the real working conditions of the GIL pipeline. We adopted the Gaussian 09 (Rev E.01) quantum chemistry package to calculate the interaction potential between N_2-N_2, N_2-SF_6, and SF_6-SF_6 molecules and fitted Lennard-Jones potential parameters under the framework of Density Functional Theory (DFT). GD3BJ dispersion interaction is added to the calculation parameters. On the mesoscopic scale, a statistical physical model of the state distribution of SF_6/N_2 mixed gas in the pipeline is established based on this microscopic model, and the Lammps (Large-scale Atomic/Molecular Massively Parallel Simulator) program package is used to simulate the performance of molecular dynamics on the micron scale. A statistical physical model of mixed gas was established on a macro scale, and the distribution of gas molecules in the GIL pipeline was analyzed. Consider the influence of pipeline properties and environmental factors in the discussion.

B. TEST PLATFORM

This paper uses the experimental setup which is shown in Figure 1 to detect the gas ratio of SF_6/N_2 mixed gas at different heights. The experimental platform is a sealed experimental tower made of welded steel plates, with a height of 30 meters and a diameter of 60 cm. First, use a high-power vacuum pump to vacuum the experimental tower to a pressure of 133Pa. According to Dalton's law of ideal gas, use the partial pressure method to prepare SF_6/N_2 mixed gas, and control the flow of SF_6 and N_2 gas through the pressure reducing valve and high-precision pressure gauge, A certain proportion of SF_6/N_2 mixed gas is prepared and the ratio of the initial mixed gas is about 2/8. The mixed gas is injected into the experimental tower from the bottom. As time goes on, the gas will be distributed throughout the experimental tower., and fill it into the experimental tower from the bottom.

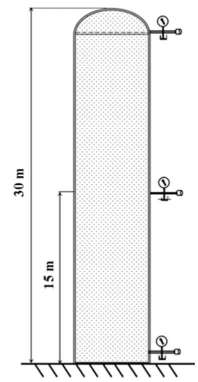

FIGURE 1. SF_6/N_2 mixed gas distribution experiment platform.

In the aspect of detection, detections port are installed the bottom, middle and upper parts of the experimental tower, respectively. A pressure gauge is installed at each port to monitor the pressure change of the mixed gas in the experimental tower in real time. The mixing ratio detector is used to regularly detect the ratio of the mixed gas.

Test gas: SF_6 gas (purity not less than 99.99%), N_2 gas (purity not less than 99.999%).

III. SIMULATION MODELING AND ANALYSIS

A. SPECIFIC INTERMOLECULAR INTERACTIONS AT THE MICROSCOPIC SCALE

By fixing the single molecular configuration and changing the intermolecular distance (along the z direction), the total energy of the system is calculated, and the molecular dissociation potential energy surface curve is obtained (as shown in Figure 2).

After applying an electric field of 0.001 au (atomic unit) along the y direction, the potential energy curve is scanned, the absolute value of the potential energy curve decreases, but the dissociation energy (potential well depth) remains basically unchanged.

Comparing the potential energy surface without electric field and considering electric field, before and after the electric field is added, the effects of electric field can be determined. The electric field mainly reduces the interactions. Among these interactions, the electric field has the most

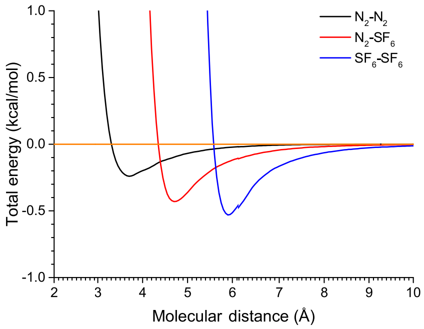

FIGURE 2. Molecular potential energy surface of N_2-N_2, N_2-SF_6, SF_6-SF_6.

effect on the energy of SF_6-SF_6, and has little effect on the energy of N_2-N_2. This is consistent with the result of the polarization rate obtained by the quantitative calculation.

$$\alpha_{N_2,yy} = 13.25\text{au}, \quad \alpha_{SF_6,yy} = 23.33\text{au}$$

By means of quantum chemical methods, the eigenvalues, average values and response coefficients of various microscopic physical quantities can be accurately calculated. In order to calculate the polarizability of the SF_6 molecule and analyze the relationship between the polarizability and the electric field strength, firstly we derive the physical meaning and mathematical formula of the induced dipole moment and polarizability of the microscopic system, then quantify it with our own program calculation and analysis. When the electric field is small, the energy obtained by the single-point calculation and the structural relaxation calculation is not much different. When the electric field approaches to 0, the polarizability tends to the calculation result of the response theory. Structural relaxation will bring great nonlinear effects.

B. INTERMOLECULAR CORRELATIONS AT THE MESOSCOPIC SCALE

In the MD simulation process, the time step is selected as 0.01 fs, and the temperature is selected as 300 K. First, relax under the NVT ensemble to make the system reach the equilibrium under the target conditions, calculate 2.0E+06 steps, and output result every 4.0E+05 steps. After equilibrium, the pressure of the system is calculated to be 0.005518, which corresponds to 0.619 MPa. Figure 3 is a typical snapshot of the particles output at the selected four moments, respectively. Although it is several times the standard atmospheric pressure in the GIL pipeline, the number density of the particles is still very small, the average distance between the particles is quite far, the interaction between each other has no effect on the statistical properties, and no correlation effect is observed between the particles, so it is still in an ideal gas state. It should be noted that the gravity of a single particle is very small, and there is basically no collision between particles. The motion of the particles can be regarded as independent of each other, so gravity will not affect the scale range (micrometer) concerned by molecular dynamics. This is mainly due to the fact that the width of the potential well (Å) that determines the attraction and

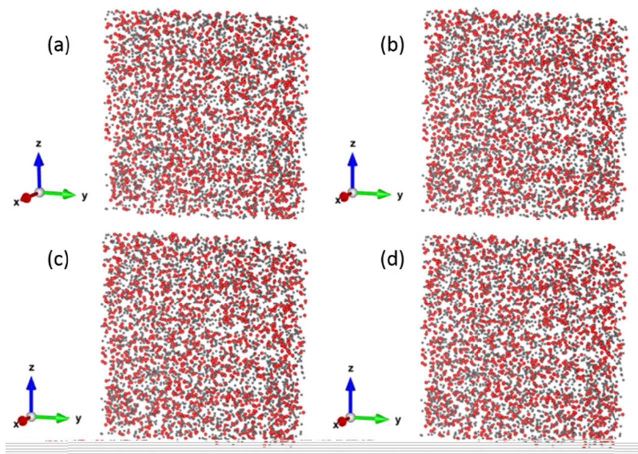

FIGURE 3. (a) Initial position type; (b) 400,000 step post position type; (c) 800,000 step post position type; (d) 1,200,000 step post position type.

interaction between molecules is too small relative to the average distance between molecules (100 Å), and the depth of the potential well is much smaller than the thermal energy from temperature in scale of k_BT. Therefore, the molecular interaction does not affect the gas distribution state under the working conditions of the GIL, and is always in a uniform distribution state on the micrometer scale.

The working temperature of GIL pipes is in the range from −20 degrees Celsius to 100 degrees Celsius. In present work, MD simulations were performed at 3 different temperatures, T=370 K, T=275K, and T=255K to mimic the working conditions. In principle, the effect of intermolecular interaction force and gravity are effectively enhanced under low temperature conditions. However, according to the present MD calculations, the characteristic length of the correlation caused by the intermolecular interaction is much smaller than the average distance of the molecule even in the case of sub-zero temperature, and the characteristic length caused by the gravitational potential energy is also much larger than the scale range that can be calculated through the molecular dynamics simulation. No intermolecular correlation behavior has been found under various temperature conditions, therefore, the mixed insulating gas can be considered an ideal gas within the temperature range of the GIL.

C. MACRO-SCALE STRATIFICATION

According to the law of air pressure in the gravity field, the distribution function of gas density with height can be expressed by,

$$n\left(h\right) = n_0 \frac{T\left(h_0\right)}{T\left(h\right)} \exp\left[-\int_{h_0}^{h} \frac{dz}{H\left(z\right)}\right], \tag{1}$$

where n(h) is the gas density at the reference height h, and T(h) is the temperature at the height h.

$$H\left(h\right) = \frac{k_B T\left(h\right)}{mg\left(h\right)}, \tag{2}$$

is called as pressure elevation in atmospheric physics. H is a parameter that is inversely proportional to molecular weight and directly proportional to temperature when considering that the acceleration of gravity and temperature do not vary with height over the length of the GIL pipeline. For the N_2 molecules studied in this work (m_{N2}=4.65 × 10.26 kg), H_{N2}=30.28T m/K; SF_6 molecules (m_{SF6}=24.26 × 10.26 kg), H_{SF6}=5.804T m/K. In the ideal gas approximation, that is, the interaction between molecules is ignored, and only the instantaneous collision between molecules is considered. The molecular dynamics calculations in the previous chapter proved that the collision between molecules can be ignored under the actual working pressure. Therefore, this formula can be expressed as,

$$n(h) = n_0 e^{-\frac{h-h_0}{H}}, \tag{3}$$

according to this expression, it can be seen that the pressure elevation is the key characteristic scale for the gas density distribution in the gravitational field, and it can be selected as the length reference unit when discussing the behavior of various gases. The characteristic length of SF_6 gas is relatively small, which may be close to 1 km in a low-temperature working environment similar to the Northeast region of China. The characteristic length of the N_2 molecule is on the order of 10 km, so the stratification is not obvious within the possible length of the pipeline.

According to the distribution function shown in the above formula, the average density in the vertically placed closed pipe with a length of L studied in this project can be expressed as

$$\bar{n} = \frac{n_0}{L}\int_0^L e^{-\frac{h}{H}} dh = \frac{n_0}{L}\int_0^L e^{-\frac{h}{H}} dh = \frac{n_0}{L} H \left(1 - e^{-\frac{L}{H}}\right), \tag{4}$$

In real working conditions, the average density in the pipeline and the height of the pipeline are certain physical quantities. According to formula (3.4), the bottom density n_0 and the top density n_L of the pipe can be expressed as a function of the average density and the pipe height:

$$n_0 = \frac{\bar{n}L}{H\left(1 - e^{-\frac{L}{H}}\right)} = \bar{n}\frac{L}{H}\left(1 - e^{-\frac{L}{H}}\right)^{-1}, \tag{5}$$

$$n_L = \frac{\bar{n}L}{H\left(e^{\frac{L}{H}} - 1\right)} = \bar{n}\frac{L}{H}\left(e^{\frac{L}{H}} - 1\right)^{-1}, \tag{6}$$

These two relations indicates a general non-uniform distribution of gas in the GIL. The density at the top of the pipe decreases rapidly as the height of the pipe increases. According to these relations, when the pipeline height L is about 10 times the pressure elevation H, when the pipeline height L is about 3.5 times the pressure elevation H, its density drops to one hundredth of the average density. When it is 1.2 times of the elevation, its concentration drops to one-half. The density change at the bottom of GIL is relatively gentle with the change of the pipe height. When the pipeline height L is about 10 times the pressure elevation H, the density at the bottom end increases by an order of magnitude.

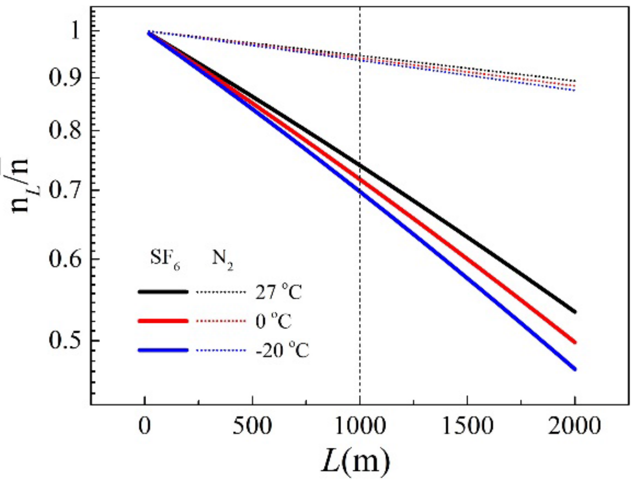

FIGURE 4. The relative average density at the top of the pipe varies with the height of the pipe when the average density is constant. Here shows the relationship of three typical temperature cases and the comparison of two kinds of molecules.

Under actual working conditions, the average density of two gas molecules is given. In this project, the influence of pipeline height on the uneven distribution of gas is considered. Under three typical temperature conditions, such as -20 degrees Celsius, freezing point temperature and 27 degrees Celsius at room temperature, the deviation behavior of the gas density at the top of the pipe from the average density can be calculated according to the formula (3.5-3.6), as shown in Figure 4.

Since $H_{SF6} \ll H_{N2}$, the effect of SF_6 molecular gravity on the density at the top of the pipe is much greater than that of N_2 molecules. It can be seen from Figure 4 that the rise of the GIL pipeline height does not change the distribution of N_2 molecules in the pipeline. For pipelines more height than 500 m, the top density decreases by less than 3%; for a 100 m high pipeline, the gravity effect can only cause a 0.5% change in N_2 gas density at the top of the pipeline. In addition, the operating temperature does not have a significant effect on this rule, and the curve of the given temperature in Figure 4 differs by less than 0.1%. Therefore, the distribution of N_2 gas in the gravity effect can be completely ignored in the process of engineering application.

The stratification of SF_6 molecules under gravity is the core issue of this work. Figure 4 is also a reference for actual engineering. According to Figure 4, SF_6 molecules will indeed cause uneven distribution of the system under the action of gravity, especially at the top of the pipe. At the top of a pipe with a height of 1000 m, the density is reduced to 30% of the average concentration and the insulation properties will be greatly reduced compared with the bottom. When the pipeline is about 310 m high, the top concentration drops to 10% of the average concentration. Because H_{SF6} is on the order of 1000 m. The influence of temperature on this gravity effect is also significant. At the top of a 100 m high pipe, a temperature difference of 20 degrees Celsius can cause a 1% difference in concentration.

TABLE 1. Changes of SF6 gas content in different parts of the experimental tower after inflation.

Detection Time	Lower Part	Central	Upper Part
1	88.1	0.3	0.0
3	84.6	3.4	0.0
7	75.0	7.1	0.3
8	73.6	8.2	0.7
15	58.8	16.8	3.7
20	52.0	22.9	4.9
24	45.6	28.0	6.3
29	40.8	33.9	7.6
36	36.1	28.1	10.3
41	32.8	24.1	11.5
50	22.1	23.2	16.5
57	19.3	20.2	18.3
65	19.3	19.5	19.5
79	19.4	19.4	19.3

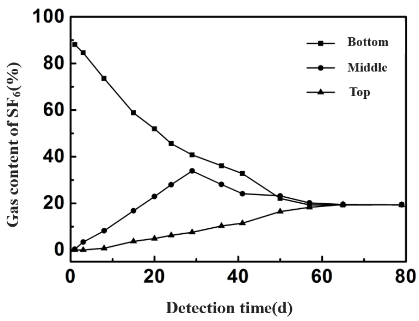

FIGURE 5. Change trend of SF_6 content.

IV. EXPERIMENTAL RESULTS AND ANALYSIS

A. THE MOVEMENT STATE OF THE SF_6/N_2 MIXED GAS IN THE EXPERIMENTAL TOWER AFTER INFLATION

After the filling of the SF_6/N_2 mixed gas, in order to explore the movement state of the mixed gas in the experimental tower, the SF_6 content in the mixed gas at different positions is regularly detected. The experimental results are shown in Table 1.

It can be seen from the experimental results, as shown in Figure 5, that 12 days after the completion of the gas inflation, the SF_6 gas content at the bottom of the experimental tower was 88%, the SF_6 gas content in the middle was 0.3%, and no SF_6 gas was detected at the top. With the continuous movement of the two gas molecules, the SF_6 gas content at the bottom gradually decreases, and the SF_6 gas content in the middle and top gradually increases. After 29 days of filling, the SF_6 gas content in the middle has an inflection point, reaching the highest value of 33.9%, and then gradually decreasing to 19.3 %, and remain unchanged; SF_6 gas was detected at top 30 meters height on the 7th day after inflation, and the SF_6 content gradually increased, and the SF_6 content stabilized after about 65 days. That is, after about 70 days after inflation, the SF_6 and N_2 gases at the top, middle, and bottom of the experimental tower were uniformly mixed, and the SF_6/N_2 mixed gas was uniformly distributed.

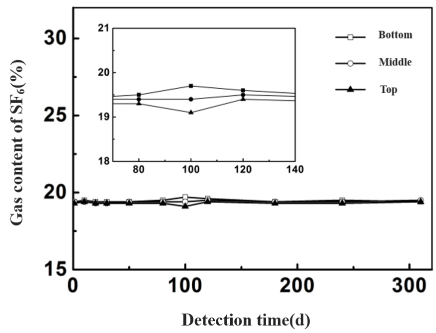

FIGURE 6. Variation trend of SF_6 content in different detection positions.

In the filling experiment, as shown in Figure 6, SF_6 gas is charged from the bottom first, and then N_2. At the initial stage of inflation, a large amount of SF_6 gas gathered at the bottom of the experimental tower, so the bottom SF_6 gas content was the highest. Subsequently, SF_6 molecules diffuse from a high concentration at the bottom of the tower to a low concentration at the top of the tower, and N_2 molecules diffuse from a high concentration at the top of the tower to a low concentration at the bottom of the tower. As the two molecules move continuously, the mixed gas in the experimental tower tends to be evenly distributed.

B. THE MOVEMENT STATE CHANGE OF THE SF_6/N_2 MIXED GAS AFTER THE GAS IS EVENLY MIXED

Explore whether it will be further stratified, after SF_6/N_2 mixed gas was evenly mixed, the change of SF_6 gas content in the experimental tower was tracked and tested for as long as one year. The experimental results are shown in Table 2.

It can be seen from the experimental results that within three months after SF_6/N_2 gas mixture is evenly mixed, the change of SF_6/N_2 gas mixture ratio at different heights is basically negligible, which can be considered that the mixed gas is uniformly distributed and stable. At other temperatures, the mixture gas composition at each part of the test tower has little change. Therefore, it can be preliminarily considered that SF_6/N_2 gas mixture has no obvious stratification within the temperature range of $0\sim40°$, and the influence of temperature on the stratification of gas mixture is negligible.

During the period of 80-120 days, the SF_6 gas content in the upper, middle and lower parts showed slight differences. The SF_6 gas content in the lower part increased while the SF_6 gas content in the upper part decreased. On the 100th day, the maximum value appeared, the lower SF_6 gas content was 19.7%, the upper SF_6 gas content was 19.2%. The fluctuation of SF_6 gas content was mainly due to the fact that it was winter in this period and the ambient temperature dropped to about 5°. On the 100th day (29 December 2018), the ambient temperature is -5 ° C and the difference between the upper and lower SF_6 gas content is 0.5%. It may be because when the temperature drops greatly, the trace amount of SF_6 at the bottom condenses and moves to the bottom of the experimental tower.

The above experiments were carried out under the condition of without electric field, and the surrounding

TABLE 2. Changes of SF_6 gas content in different parts of the experimental tower after uniform mixing.

Detection time	Lower part	Central	Upper part
1	19.4	19.4	19.3
10	19.4	19.4	19.4
20	19.4	19.3	19.4
30	19.4	19.3	19.4
50	19.4	19.4	19.3
80	19.5	19.4	19.3
100	19.7	19.4	19.2
120	19.6	19.5	19.4
180	19.4	19.4	19.3
240	19.4	19.4	19.3
310	19.4	19.4	19.4

environment of the GIL equipment on site is complex, especially the ambient temperature may affect the stratification of the mixed gas. For the GIL pipeline, the temperature of the surrounding air does not exceed 40°, and the temperature of the intermediate conductive rod generally does not exceed 105°. There is a temperature difference of about 60° in the pipeline. That is, conductors heat steadily, pipes lose heat steadily to the environment, there is a steady temperature gradient, and the gas conducts heat. The temperature difference leads to heat transfer and accelerates the diffusion movement of molecules. In other words, the greater the temperature difference is, the better the movement of molecules will be, and the smaller the possibility of SF_6/N_2 gas mixture stratification is.

V. CONCLUSION

From quantum chemical calculations of microscopic molecular interactions, to molecular dynamics simulations, and macroscopic statistical mechanical analysis. The mixed gas stratification only has a significant impact on the vicinity of the top of the pipeline when the height of the pipeline is close to the order of 1 km, which is reflected in the decrease of the density at the top relative to the average density in the pipeline. The solution is to reduce the length of the pipeline. In addition, the temperature of the working environment will also have an effect on the segmentation. The lower the temperature, the more obvious the dispersion. Taking into account the gas stratification problems caused by gravity and low-temperature SF_6 gas condensation, from engineering considerations, the heating device can be installed at an appropriate location to reduce the possibility of condensation and promote the movement of the gas to help the mixed gas maintain a balance in the space. The observed result is that the mixed gas that has experienced heat equilibrium will not occur breakdown accidents due to stratification problems in engineering applications.

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