IEEE Access
Multidisciplinary | Rapid Review | Open Access Journal

Received December 17, 2020, accepted January 11, 2021, date of publication January 18, 2021, date of current version January 25, 2021.

Digital Object Identifier 10.1109/ACCESS.2021.3052060

Investigation on Diffusion Mechanisms of Methanol in Paper/Oil Insulation Based on Molecular Dynamics Simulation

XIANHAO FAN[1], (Student Member, IEEE), HUAN ZHAO[1], TENGYUE SUN[1], JIEFENG LIU[1], (Member, IEEE), YIYI ZHANG[1], (Member, IEEE), AND YUBO ZHANG[2]

[1]Guangxi Key Laboratory of Power System Optimization and Energy Technology, Guangxi University, Nanning 530004, China
[2]Electric Power Research Institute, Guangxi Power Grid Company Ltd., Nanning 530023, China

Corresponding author: Jiefeng Liu (liujiefeng9999@163.com)

This work was supported in part by the National Natural Science Foundation of China under Grant 51867003 and Grant 52007036, in part by the Natural Science Foundation of Guangxi under Grant 2018JJB160064 and Grant 2018JJA160176, in part by the Guangxi Bagui Young Scholars Special Funding, in part by the Boshike Award Scheme for Young Innovative Talents, in part by the Guangxi Key Laboratory of Power System Optimization and Energy Technology Project under Grant AE3020001829, in part by the Guangxi Science and Technology Base and Talent Special Project under Grant 2019AC20096, and in part by the Basic Ability Improvement Project for Young and Middle-aged Teachers in Universities of Guangxi under Grant 20190067 and Grant 20190046.

ABSTRACT Methanol is regarded as an available indicator to analyze the aging condition of cellulose insulation. However, the diffusion mechanism of methanol molecules in the paper-oil insulation system is still unclear, since it cannot be explored by using only experiments. Given this issue, the molecular dynamics simulations were performed to investigate the diffusion mechanism of methanol molecules. In the current work, the mean square displacement of methanol during the diffusion process was calculated and analyzed, as well as its trajectory tracking. Then, the research on interaction energies and hydrogen bonds in paper/oil system were conducted. Finally, the effect of temperature on the diffusion of methanol molecules was also studied. Findings revealed that the diffusion of methanol in cellulose insulation is faster than that in insulating oil, besides, the presence of hydrogen bonds affects the diffusion rate of methanol molecules in cellulose insulation and insulating oil. Thus, the present findings could support the investigation of the diffusion mechanisms of methanol molecules, by which the aging condition evaluation of cellulose insulation could be also promoted.

INDEX TERMS Cellulose insulation, diffusion mechanisms, methanol, molecular dynamics simulation.

I. INTRODUCTION

The service life of an oil-immersed transformer is determined by the performance of its paper insulation [1]–[3]. Due to the excellent electrical and mechanical properties, cellulose (crucial material of paper insulation) has been utilized in oil-immersed transformers for more than 100 years. The average length of cellulose chains is defined as the viscometric degree of polymerization (DP_v), which is regarded as an important parameter for reflecting the mechanical property of cellulose. Consequently, the application of DP_v could promote the lifespan determination of the transformer. However, the running transformer needs to be de-energized to sample the cellulose insulation for measuring its DP_v. It is thus rather impractical for field testing on real transformers. In comparison, it is easier to obtain samples of insulating oil from the transformers in service [4]. Thus, if the relationship between the aging degree and the oil-soluble indicator related to the aging of cellulose insulation could be established, it would be beneficial for degradation assessment by using insulating oil.

In the 1980s, carbon oxides (CO and CO_2) were put forward as the specific indicator [5]. Nevertheless, the application of carbon oxides is limited considering that they could be generated not only from the aging of cellulose insulation but also from the long-term oxidation of insulating oil [6]. A few years later, Burton *et al.* [7] proposed a family of furan compounds to assess the aging condition of cellulose insulation aging. Unlike carbon oxides, the production of these furan compounds is solely related to the degradation of cellulose insulation. However, the most abundant furan

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

compound detected in insulating oil, i.e. 2-furfuraldehyde (2-FAL), generates not only from the breakdown of α-cellulose but also from hemicellulose degradation [8]. Also, 2-FAL can hardly be detected when the cellulose insulation is thermally upgraded (TU) Kraft paper, which is used in a high percentage of modern transformers [9]. In this case, the use of 2-FAL as an aging indicator is also limited. However, it was verified that methanol can be used to access the ordinary Kraft paper, as well as thermally upgraded Kraft paper. Besides, methanol can rapidly re-equilibrate with the oil after oil intervention like oil degassing or regeneration, since it has a high affinity with cellulose [10], [11]. Therefore, methanol has been proposed as a new aging indicator for characterizing the aging of cellulose [9], [12].

The concentration of indicator (methanol) in insulating oil is rather important for electric utilities to determine whether the tested unit should be replaced [10], [11]. Due to the diffusion behavior of the aging indicator (methanol) is related to the concentration of indicator in insulating oil, the laboratory experiments on the diffusion of methanol molecules in cellulose were thus carried out [10], [11]. It was reported that the time for 2-FAL to recover its initial concentration after insulation oil regeneration is twice that of methanol [10].

Although the diffusion activities have been preliminarily explored by several experiments, the diffusion mechanisms at molecular and atomic levels have still not been fully studied. Such a situation is attributed to the fact that the diffusion mechanism cannot be interpreted by using only experiments. Consequently, further studies for exploring the diffusion property of methanol are required. It is worth noting that findings pointed out that molecular dynamics simulations could be utilized to study diffusion property and even mechanisms [13]–[15], by which the obtained results will consistent with the actual experiments. Since molecular dynamics simulations can support detailed microscopic modeling at the molecular and atomic scale combining electricity, physics, chemistry, and other disciplines [16], [17], the research of diffusion mechanisms of methanol at atomic and molecular levels thus could be achieved by using molecular dynamics simulations.

Given this purpose, molecular dynamics simulations were performed to study the diffusion mechanisms of methanol molecules in the paper-oil insulation system. In the present work, the mean square displacement (MSD) of methanol molecules was calculated, which indicated that the diffusion of methanol molecules in insulating oil is more obvious than that in cellulose. The trajectory tracking of the centroid of methanol molecules indicated that methanol has a high affinity for cellulose. The existence of a large number of hydrogen bonds between cellulose and methanol molecules suppress the diffusion of methanol in cellulose. In addition, the temperature effect on diffusion behavior was investigated—the effect of temperature on the diffusion of methanol molecules in insulating oil is greater than that in cellulose. Thus, the present findings are expected to provides support for studying the diffusion mechanism of methanol molecules, which is valuable for the aging condition evaluation of cellulose insulation.

II. DIFFUSION PRINCIPLE

The *MSD* indicates the position deviation of a particle corresponding to a reference position over time [18], [19], which is an important parameter to characterize the diffusion behavior [20]. The *MSD* at time t is defined as an ensemble average, as shown in Equation (1).

$$MSD = \left\langle |x(t) - x(0)|^2 \right\rangle = \frac{1}{N} \sum_{i=1}^{N} |x^{(i)}(t) - x^{(i)}(0)|^2 \quad (1)$$

where *MSD* is the mean square displacement; $x^{(i)}(t)$ is the position of the i-th particle at time t; $x^{(i)}(0)$ represents the reference position of the i-th particle.

The linear relationship between the *MSD* and simulation time can reflect the information corresponding to the diffusion coefficient [21]. In general, the diffusion coefficient is defined as the ratio of flux density to the negative number of the concentration gradient in the diffusion direction. In molecular dynamics simulation, the relationship between the *MSD* and the diffusion coefficient can be expressed by using the Einstein relation, which is shown in Equation (2).

$$D = \frac{1}{6N} \lim_{t \to \infty} \frac{d}{dt} \sum_{i=1}^{N} \left\langle |\vec{r_i}(t) - \vec{r_i}(0)|^2 \right\rangle \quad (2)$$

When the *MSD* is linear with time, the slope of the MSD curve over time is proportional to the diffusion coefficient. The derivation of this equation was given by Frenkel and Smit [21].

III. CALCULATION METHOD

A. MODELING

In this study, the Accelrys Materials Studio (MS) software was used to study the diffusion mechanisms of methanol molecules in the paper-oil insulation system. The Amorphous Cell module in the MS was used to build 3D periodic amorphous structures. In addition, the Forcite module in the MS was used to perform geometry optimization, energy calculations, and dynamics simulations.

1) OIL MODEL

The mineral oil is widely used as insulating oil in the paper-oil insulation system due to its high efficiency, good thermal cooling capacity, low cost, and good pouring point at low temperatures. Liu and Xu [22] analyzed the constituents of 25# mineral oil produced by the Xinjiang Karamay Petrochemical Plant in China. The results indicated that approximately 88.6% of the mineral oil is composed of alkanes and cycloalkanes, as shown in Table 1. Thus, alkanes and cycloalkanes, which mainly determine the chemical properties of insulating oil, were used to construct the insulating oil model in this study. Relevant chemical formulas and molecule

TABLE 1. Constituents of insulating oil.

Alkanes	Cycloalkanes			
	77% (w/w)			
11.6% (w/w)	One ring	Two rings	Three rings	Four rings
	15.5%	28.5%	23.3%	9.7%

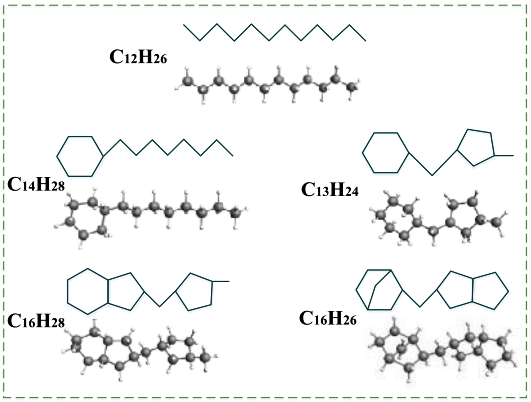

FIGURE 1. Chemical formulas and molecule models of mineral oil constituents. (Color code: carbon atom-gray, hydrogen atom-white).

models of mineral oil constituents were built and shown in Fig. 1.

2) CELLULOSE MODEL

Cellulose consists of the repeating unit of cellobiose [23], [24], as shown in Fig. 2. Native cellulose has two different morphologies, namely, amorphous region and crystalline region. The crystalline region mainly contains ordered cellulose molecules, while the amorphous region is typically composed of irregularly arranged molecules. Considering that the crystalline region is expected to gradually turn into an amorphous state at high temperatures [25], the crystalline region is excluded in this paper. Different degrees of polymerization have little effect on molecular conformation or physicochemical properties [26], especially when studying the adsorption and diffusion of an object [27]. Thus, with the consideration of computational power and efficiency, cellobiose was used as a repeating unit to build the amorphous region model.

3) PAPER-OIL INTERFACE MODEL

When the initial models are completed, the Build Layers tool was used to construct a paper-oil interface. It was reported that the density of insulating oil is around 0.8-0.87 g/cm^3 [28]. In this paper, the 3D periodic amorphous structure of insulating oil with a density of 0.87 g/cm^3 was built for molecular dynamics simulations. According to research [27], [29], the model of cellulose with a density of 1.5 g/cm^3 was built. Considering that methanol molecules are mainly produced by the aging of cellulose insulation, the methanol molecules are initially distributed in the model

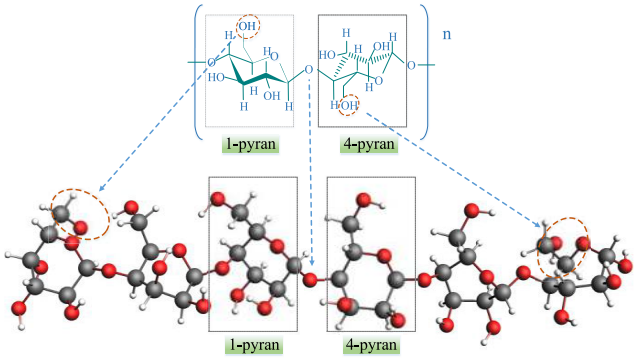

FIGURE 2. Chemical formula and molecular model of cellobiose. (Color code: hydrogen atom-white, carbon atom-gray, and oxygen atom-red).

of cellulose. Detailed steps of the simulation were illustrated in Fig. 3.

B. SIMULATION DETAILS

The PCFF force field used in this study is suitable for geometry optimization and molecular dynamics simulation of carbohydrates [30], [31]. Since the initial model of the paper-oil insulation interface was unstable, geometry optimization was performed in the Forcite module to optimize the system. To realize full optimization, the maximum number of optimization iteration was set to 5000, after which the potential energy of the system tended to be a constant (Fig. 4).

The high temperatures can provide enough energy to the simulation system for overcoming the energy barrier and finding the lowest point of energy. Therefore, annealing was carried out at a temperature of 300-1000 K with an interval of 100 K. The energy optimization was conducted in each annealing process. Dynamics simulations were carried out after the optimization. The simulations were controlled by a canonical ensemble in which the substance, volume, and temperature remain unchanged (i.e. the NVT ensemble). The intensity of standard atmospheric pressure (0.1 Mpa) was used. The temperature was controlled through the Anderson algorithm [32].

For a given temperature, the new velocity is given by Maxwell-Boltzmann statistics based on the reassignment of the velocity of selected atoms or molecules. In this study, the atom motion was updated every 3000 steps at a time interval of 1 fs, which meant a frame was output every 3 ps. Each molecular dynamics simulation lasts 600 ps. To ensure the accuracy of the calculation, each simulation was performed ten times, and the average values of the calculation were taken.

IV. RESULTS AND DISCUSSION

A. DIFFUSION OF METHANOL IN CELLULOSE AND INSULATION OIL

Molecular dynamics simulation was carried out to calculate the MSD of methanol molecules in cellulose and insulating oil. The temperature was set to 343 K, which corresponds to the service temperature of transformers. The results were

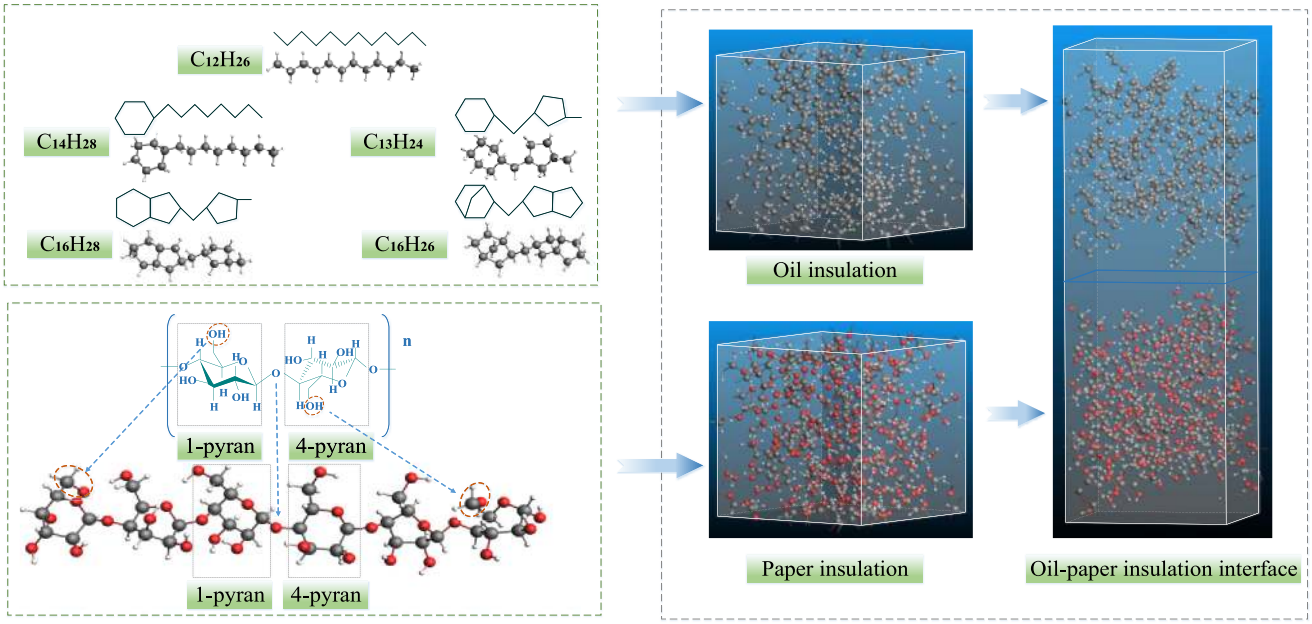

FIGURE 3. Flow diagram of the simulation. (Color code: hydrogen atom-white, carbon atom-gray, and oxygen atom-red).

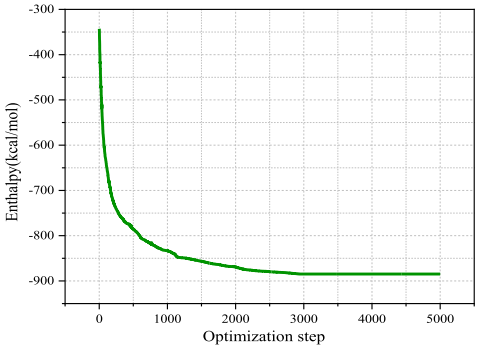

FIGURE 4. The changes in potential energy over optimization steps.

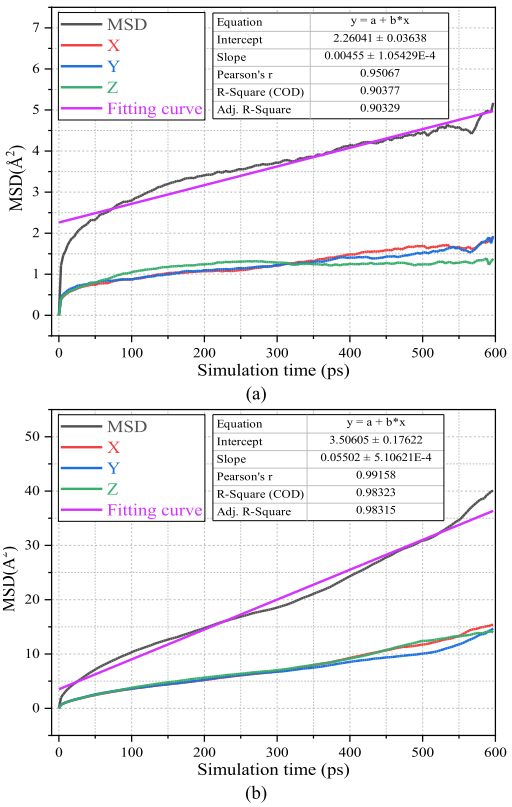

FIGURE 5. The MSD of methanol molecules (a) in the cellulose model and (b) in the insulating oil model.

shown in Fig. 5. Black curves in Fig. 5a and Fig. 5b represent the changes in MSD of methanol molecules versus simulation time, respectively.

In the beginning, the increase of MSD is rapid, which is attributed to the rapid increase in simulation temperature. After approximately 25 ps, the diffusion of methanol reaches equilibrium, and the MSD of methanol molecules is linear with the simulation time. The linear relationship suggests that the diffusion of methanol molecules has reached equilibrium and began to diffuse uniformly. According to the fitting curves (purple lines in Fig. 5), the slope of the MSD curve of methanol in insulating oil is larger than that in cellulose, which indicates that the diffusion coefficient in insulating oil is larger than that in cellulose. It can be concluded that the diffusion of methanol molecules in insulating oil is faster than that in cellulose.

In addition, the trend of MSD in the X (the red curve), Y (the blue curve), and Z (the green curve) directions are similar, regardless of whether the methanol is in cellulose (Fig. 5a) or insulating oil (Fig. 5b). Therefore, the diffusion of methanol in cellulose and insulating oil is isotropic. Fig. 6 shows the MSD of methanol molecules in models of the paper-oil insulation system calculated at 343 K. The change of the MSD (the black curve) can be divided into three stages. From the beginning to about 25 ps, the MSD has increased

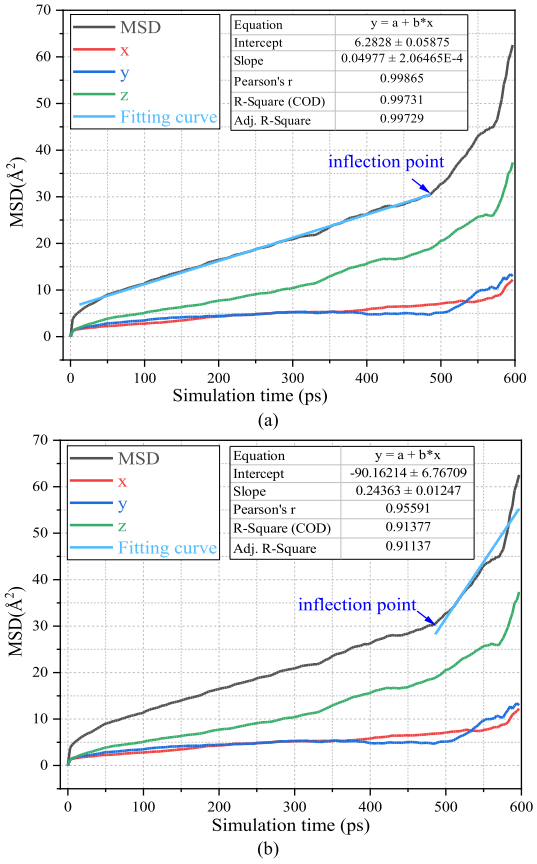

FIGURE 6. Changes in the MSD of methanol molecules in the paper-oil interface. (a) Linear fit before the inflection point; (b) Linear fit after the inflection point.

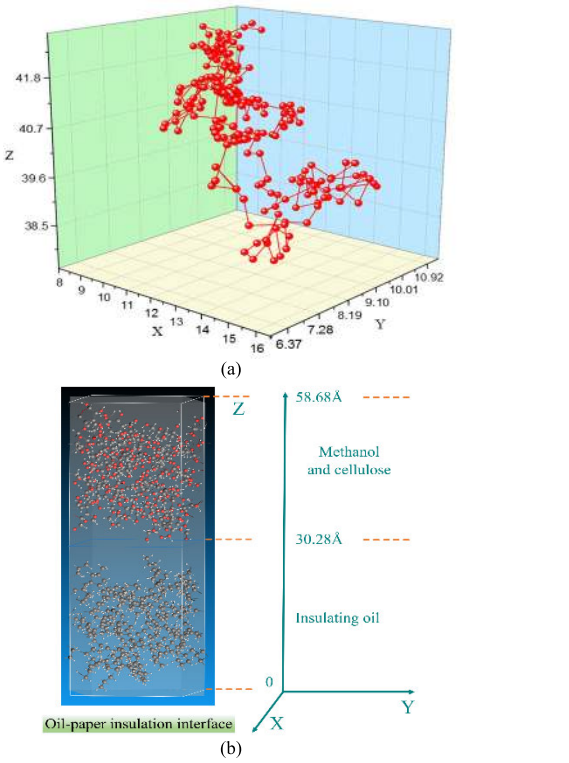

FIGURE 7. The centroid trajectory of all methanol molecules in the model of paper-oil interface. (a) The detailed trajectory of the centroid; (b) The coordinates of the paper-oil insulation model.

sharply. As mentioned before, this section is mainly affected by the rapid increase of simulation temperature, which is ignored in the following analysis. Then, the increase rate tends to be moderate in the second section, which implies the diffusion of methanol molecules mainly exists in cellulose at the beginning of simulation.

When an inflection point occurs at around 483 ps, the MSD increases rapidly. The inflection point may be attributed to the diffusion of a certain amount of methanol molecules from cellulose to insulating oil. Besides, the MSD component in the Z direction (the green curve) corresponding to the direction of the paper-oil interface is significantly greater than that in the X direction (the red curve) and the Y direction (the blue curve). The results imply that the diffusion of methanol molecules in the paper-oil insulation system is anisotropic.

According to the MSD of methanol molecules in cellulose and insulating oil, a considerable amount of methanol molecules may remain in cellulose during cellulose aging. The Perl script in the MS was used to track the centroid trajectory of all methanol molecules in the oil-paper interface, and results are displayed in Fig. 7.

It is interesting to note that the centroid coordinates of all methanol molecules vary from 30.28 to 58.68 Å in Fig. 7a corresponding to the range of cellulose coordinates in Fig. 7b. Thus, a considerable amount of methanol molecules remains in cellulose during cellulose aging. This confirms the high affinity of methanol for cellulose proposed by Bare and Merritt [9]. Although the centroid of all methanol molecules remains in cellulose, it does not mean that no methanol molecules diffuse into the insulating oil.

To further illustrate this phenomenon, the relative concentration of methanol molecules along with the direction of the paper-oil interface is illustrated in Fig. 8.

The X-axis (corresponding to the Z coordinate of Fig. 7b) is used to distinguish the interface of cellulose and insulating oil. The Y-axis corresponds to the relative concentration of methanol molecules. The yellow part on the left section with the X coordinate range of 0 to 30.28 Å represents insulating oil, and the green part on the right section with the X coordinate range of 30.28-58.68 Å represents cellulose. As shown in Fig. 8a, there is no methanol molecule in insulating oil at the beginning of molecular dynamics simulation. After 600 ps, a detectable amount of methanol molecules occurs in insulating oil (Fig. 8b). The increase of relative concentration of methanol molecules indicated that a certain amount of methanol molecules will diffuse from cellulose to insulating oil during the simulation.

B. ANALYSIS OF AFFINITY OF METHANOL FOR CELLULOSE

As mentioned before, methanol molecules have a high affinity for cellulose, which makes the diffusion of methanol molecules in insulating oil faster than that in cellulose.

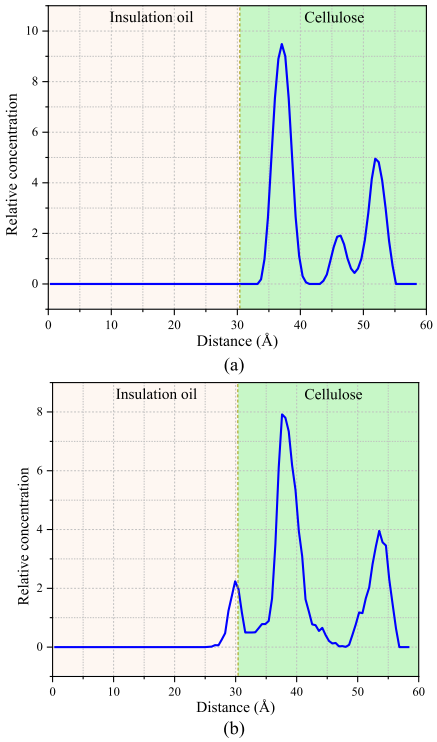

FIGURE 8. The relative concentration of methanol along with the direction of the paper/oil interface. (a) Before the molecular dynamics simulation; (b) After molecular dynamic simulation.

TABLE 2. Interaction energies between methanol molecules and cellulose and insulating oil (kcal/mol).

Interaction energies	Methanol-cellulose	Methanol-oil
ΔE	-77.67	-21.80
ΔE_{vdW}	77.14	-17.28
$\Delta E_{electrostatic}$	-111.69	-0.57
$\Delta E_{H\text{-}bond}$	-38.65	0.00

To further analyze the affinity mechanism, we calculated the interaction energy between cellulose and methanol molecules. The interaction energy is one of the important parameters to characterize the diffusion behavior of methanol molecules in cellulose and insulating oil. For brevity, the model containing cellulose and methanol is named Model 1, and the model containing insulating oil and methanol is named Model 2. Changes in interaction energies during molecular dynamics simulation are shown in Fig. 9. To further analyze the interaction energy in Model 1 and Model 2, the average interaction energies are shown in Table 2.

As we know, if there is no interaction between the substances, $\Delta E = 0$. If there is a repulsive interaction, $\Delta E > 0$. If there is an attractive interaction, $\Delta E < 0$. In the two models, the total interaction energy (ΔE) is less than zero, which indicates that the interaction of cellulose and methanol and the interaction of insulating oil and methanol are both attractive.

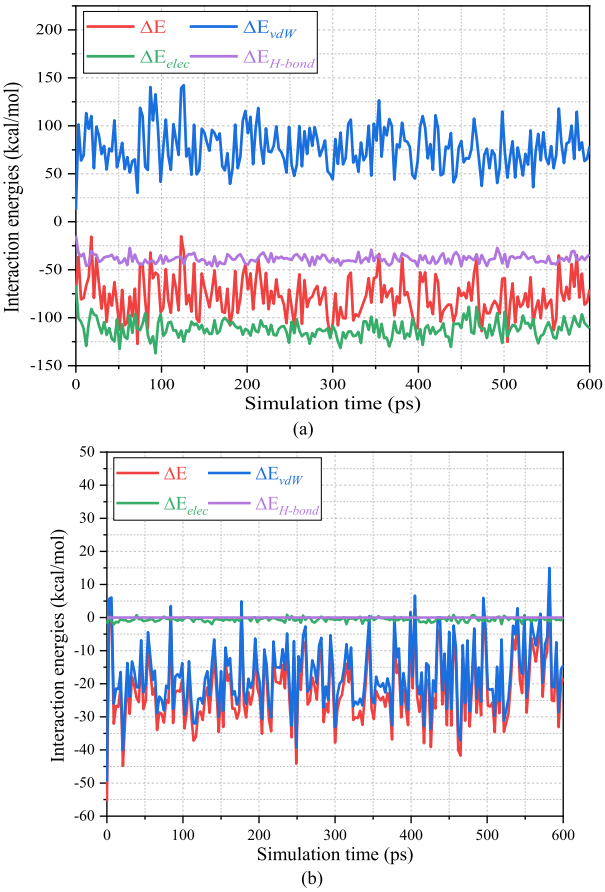

FIGURE 9. Changes in interaction energies with simulation time. (a) Model 1; (b) Model 2.

As shown in Fig. 9 and Table 2, different components of interaction energy (i.e., ΔE_{H-bond}, ΔE_{vdW}, $\Delta E_{electrostatic}$) contribute differently to the total interaction energy. In Model 1, the van der Waals force is mainly manifested as a repulsive effect. The hydrogen bonds and the electrostatic effect have significant contributions to the total interaction energy in Model 1. On the contrary, the interaction of insulating oil and methanol is mainly attributed to the van der Waals force rather than the hydrogen bonds and electrostatic effect in Model 2. In addition, the total interaction energy (ΔE) of Model 1 is more than three times that of Model 2. The results show that the interaction between cellulose and methanol is stronger than the interaction between insulating oil and methanol.

Since hydrogen bonds have contributed greatly to the attractive interaction between cellulose and methanol, we have analyzed the hydrogen bonds in this study. The hydrogen bond is defined as a special bonding interaction between a highly electronegative atom (particularly nitrogen, oxygen, or fluorine) and a hydrogen atom [33]. One methanol molecule contains a hydroxyl group, which makes it easy to form hydrogen bonds with other molecules.

According to the simulation results, the hydrogen bonds between methanol molecules and cellulose can be classified into two categories. Fig. 10a and Fig. 10b shows the first

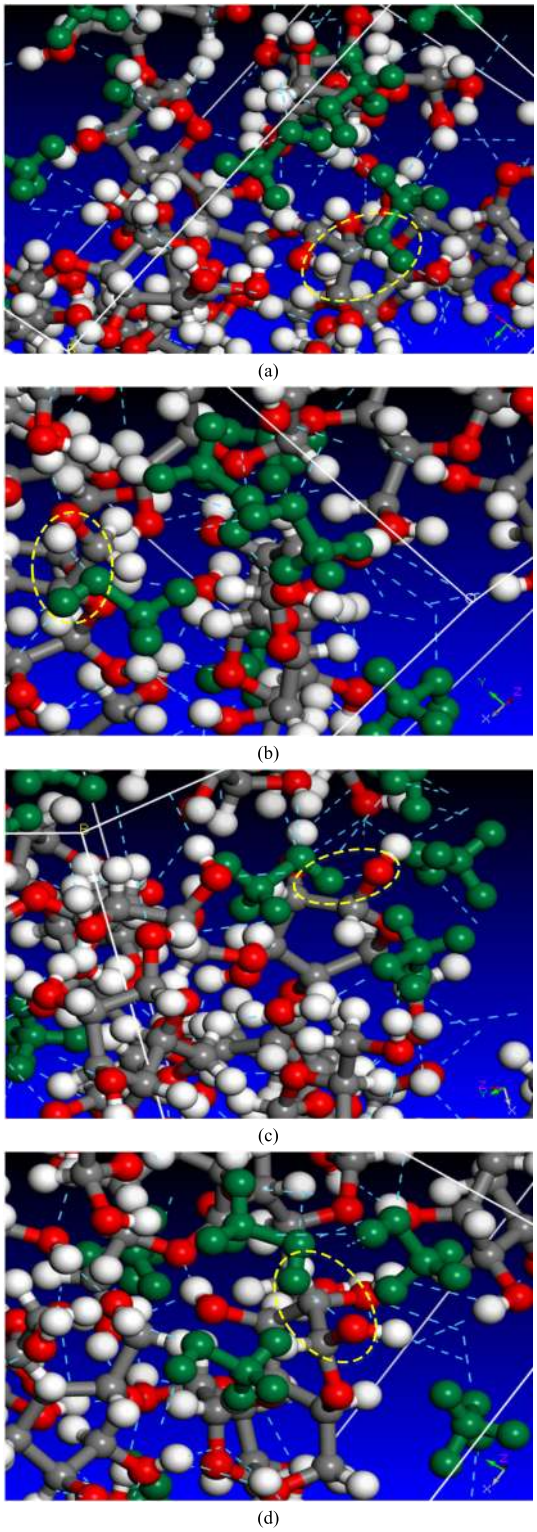

FIGURE 10. Two categories of hydrogen bonds between methanol molecules and cellulose. (a) and (b) is the first category; (c) and (d) is the second category.

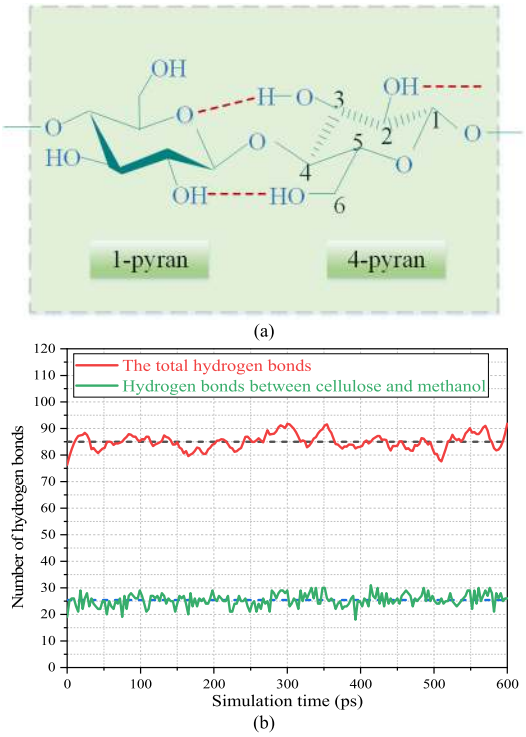

FIGURE 11. The hydrogen bonds of cellulose. (a) The location of intramolecular hydrogen bonds of cellulose molecules. (b) Changes in the number of hydrogen bonds in Model 1.

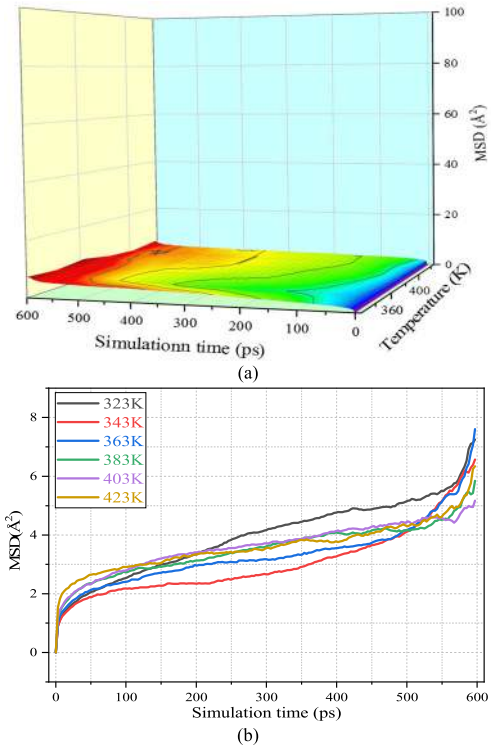

FIGURE 12. Changes in MSD of methanol in cellulose. (a) Presented in 3D; (b) Presented in 2D.

category—the oxygen atom of the hydroxyl group on the methanol molecule forms a hydrogen bond with the hydrogen atom of the hydroxyl group on cellulose. Fig. 10c and Fig. 10d shows the second category—the hydrogen atom of the hydroxyl group on the methanol molecule forms a hydrogen bond with the oxygen atom of the hydroxyl group on cellulose.

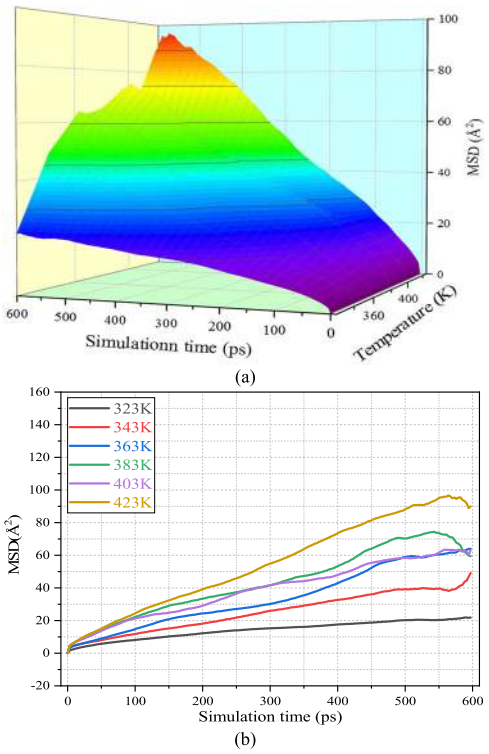

FIGURE 13. Changes in MSD of methanol in oil. (a) Presented in 3D; (b) Presented in 2D.

Hydrogen bonds in cellulose are divided into the intramolecular hydrogen bonds and intermolecular hydrogen bonds. As shown in Fig. 11a, the intramolecular hydrogen bonds of cellulose molecules are mainly formed at -OH of C-2, C-3, and C-6, as well as the O in the neighboring ring [34].

The intermolecular hydrogen bonds of cellulose molecules is mainly formed at -OH of C-2, C-3, and C-6 [34]. In this paper, the number of hydrogen bonds in Model 1 were calculated and shown in Fig. 11b. In Model 1, the total number of hydrogen bonds fluctuates around 85 (the red curve in Fig. 11b) and the number of hydrogen bonds between cellulose and methanol fluctuates around 25 (the green curve in Fig. 11b). However, from Table 2, there is almost no hydrogen bond in Model 2. Thus, it can be concluded that the presence of hydrogen bonds enhance the attractive force between cellulose and methanol molecules. As a result, the diffusion of methanol in cellulose is inhibited by these hydrogen bonds. Thus, the diffusion of methanol molecules in insulating oil is faster.

C. EFFECT OF TEMPERATURE ON DIFFUSION OF METHANOL IN CELLULOSE AND INSULATING OIL

To further investigate the diffusion mechanism, the MSD of methanol in cellulose and insulating oil was investigated at different temperatures. Fig. 12 and Fig. 13 show the MSD of methanol molecules versus simulation time at different temperatures in cellulose and insulating oil, respectively.

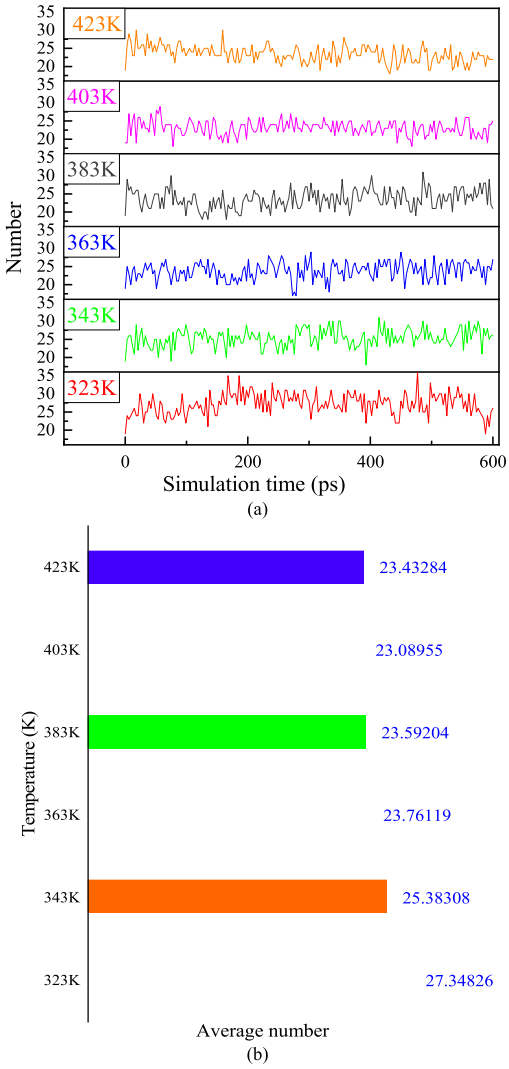

FIGURE 14. The number of hydrogen bonds between methanol molecules and cellulose. (a) Change in the number of hydrogen bonds with simulation time during molecular dynamics simulation; (b) The average number of hydrogen bonds at different temperatures.

As seen from Fig. 12a and Fig. 13a, it can be intuitively observed that the mean square displacement of methanol in insulating oil is significantly greater than that in cellulose. In Fig. 12b and Fig. 13b, the diffusion of methanol molecules reaches equilibrium rapidly after a short period. After that, the MSD of methanol molecules increases linearly under different temperatures. It is interesting to note that the effect of temperature on the MSD of methanol in cellulose is not obvious compared with that in insulating oil.

To verify the hypothesis and investigate the influence mechanism of temperature, we calculated the interaction energies between methanol and cellulose and insulating oil, and the results are shown in Table 3 and Fig. 15.

As seen from Fig. 15a, it can be intuitively observed that all interaction energies in the methanol-cellulose system remain almost unchanged under different temperatures. In Fig. 15b, the van der Waals force significantly contributes to the total interaction energy between methanol and

TABLE 3. Interaction energies between methanol and cellulose and insulating oil at different temperatures (kcal/mol).

Temperature	Methanol-cellulose				Methanol-oil			
	ΔE	ΔE_{vdW}	$\Delta E_{electrostatic}$	$\Delta E_{H\text{-}bond}$	ΔE	ΔE_{vdW}	$\Delta E_{electrostatic}$	$\Delta E_{H\text{-}bond}$
323 K	-77.63	81.62	-117.97	-41.28	-22.46	-21.84	-0.62	0.00
343 K	-73.20	77.14	-111.69	-38.65	-17.85	-17.28	-0.57	0.00
363 K	-74.04	94.15	-125.44	-42.75	-14.43	-13.86	-0.57	0.00
383 K	-71.89	79.98	-113.01	-38.86	-14.17	-13.70	-0.47	0.00
403 K	-68.80	92.81	-120.72	-40.89	-12.78	-12.30	-0.48	0.00
423 K	-75.67	79.52	-115.00	-40.19	-11.7	-11.17	-0.53	0.00

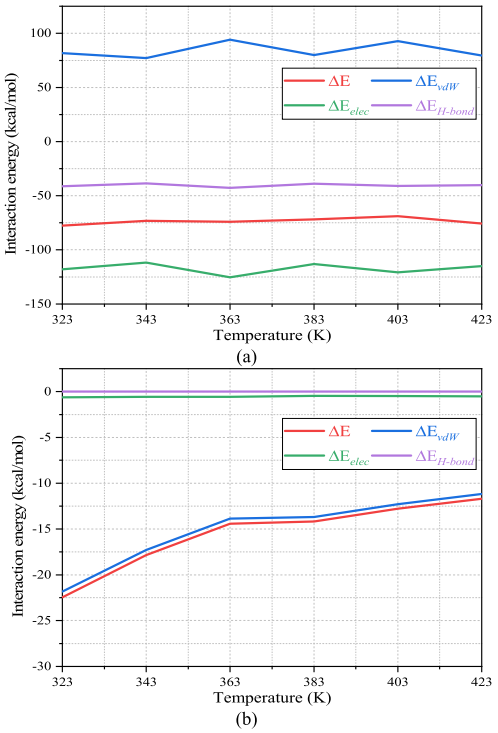

FIGURE 15. Changes in interaction energies with temperature. (a) Interaction energies between methanol molecules and cellulose; (b) Interaction energies between methanol and insulating oil.

insulating oil. As the temperature increases, the attractive van der Waals force is greatly affected by temperature and decreases sharply, which makes the attractive interaction weaker (the blue curve and the red curve in Fig. 15b).

Therefore, it leads to a more obvious effect of temperature on the diffusion of methanol in insulating oil. To further study why temperature has no obvious effect on the diffusion of methanol in cellulose paper, hydrogen bonds between cellulose and methanol molecules were calculated with a temperature range of 323-423 K. The simulation lasted 600 ps. Fig. 14a presents the changes in the number of hydrogen bonds versus simulation time during molecular dynamics simulation.

It can be observed that the number of hydrogen bonds fluctuates within a small range (from 17 to 36) regardless of temperature. The average number of hydrogen bonds between methanol molecules and cellulose at different temperatures was calculated (Fig. 14b). It can be seen from Fig. 14b that the average number of hydrogen bonds decreases by only about 4 when the temperature is increased from 323 K to 423 K. The results indicate that the influence of temperature on the number of hydrogen bonds is limited. Thus, the interaction energy contributed by the hydrogen bonds (ΔE_{H-bond}) may remain almost unchanged under different temperatures.

V. CONCLUSION

In this paper, the diffusion mechanism of methanol molecules in insulating oil and insulating oil was investigated at atomic and molecular levels by using the method of molecular dynamics simulations.

The obtained results can provide a theoretical basis for further studies of the aging analysis of cellulose. The present findings and analysis lead to the following conclusions.

I. The mean square displacements of methanol molecules in cellulose insulation and insulating oil were calculated, and the results indicated that the diffusion of methanol molecules in insulating oil is faster than that in cellulose insulation.

II. The trajectory tracking of the centroid of all methanol molecules was given, which pointed out that methanol has a high affinity for cellulose. This affinity property facilitates methanol molecules to re-equilibrate with the oil after oil regeneration.

III. The interaction energies and hydrogen bonds were calculated to study the different diffusion mechanism of methanol in cellulose insulation and insulating oil, which revealed that the presence of hydrogen bonds prevents the diffusion of methanol molecules in cellulose insulation and insulating oil.

IV. According to the mean square displacements of methanol molecules in cellulose insulation and insulating oil at different temperatures, the effect of temperature on diffusion of methanol molecules in insulating oil is greater than that in cellulose insulation. Since the van der Waals force between methanol molecules and insulating oil is greatly affected by temperatures.

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