

Article

# The Effect and Associate Mechanism of Nano SiO<sub>2</sub> Particles on the Diffusion Behavior of Water in Insulating Oil

Wenxin Tian <sup>1</sup>, Chao Tang <sup>1,\*</sup> , Qian Wang <sup>2</sup>, Shiling Zhang <sup>2</sup> and Yali Yang <sup>1</sup>

<sup>1</sup> College of Engineering and Technology, Southwest University, Chongqing 400715, China; 13657601997@163.com (W.T.); Z372475575@163.com (Y.Y.)

<sup>2</sup> Electric Power Research Institute of State Grid Chongqing Electric Power Company, Chongqing 401123, China; wangq239@163.com (Q.W.); 13243524193@163.com (S.Z.)

\* Correspondence: tangchao\_1981@163.com; Tel.: +86-23-6825-1265

Received: 9 October 2018; Accepted: 21 November 2018; Published: 26 November 2018



**Abstract:** Moisture has a significant effect on the internal insulation performance of transformers, and is closely related to the breakdown voltage of transformer insulating oil. In the present work, we studied the effect of nano-SiO<sub>2</sub> particles on the diffusion of water in insulating naphthenic mineral oil using molecular dynamics simulation. Six models were established, three of which contained nano-SiO<sub>2</sub> particles together with water concentration of 1 wt.%, 2 wt.%, or 3 wt.%. For each model variations in free volume, mean square displacement, and interaction energy were assessed. The addition of nano SiO<sub>2</sub> particles was found to reduce the free volume fraction of the model and as well as the free motion of water molecules in the oil. These particles also increased the interaction between the oil and water molecules, indicating that insulating oil containing nano-particles has a greater binding effect on water. The diffusion coefficient of water in oil containing nano-SiO<sub>2</sub> particles was reduced, such that water molecules were less likely to diffuse. The results also show that these particles adsorb water molecules in the oil and to reduce diffusion. Consequently, the addition nano-scale SiO<sub>2</sub> particles could potentially improve the breakdown voltage of the insulating oil.

**Keywords:** insulating oil; molecule simulation; nano-SiO<sub>2</sub>; free volume; interaction energy; diffusion coefficient

## 1. Introduction

With the rapid development of China's power industry, transformers have become vital components of the power transmission system. The internal insulation of these transformers is based on oil that gradually deteriorates due to many factors during prolonged use, resulting in a decrease in the insulating performance of the oil. This loss of performance is partly associated with increased water levels in the oil, together with other impurities. In the presence of an electric field, the so-called 'small bridge' effect of such impurities will render the insulating oil more vulnerable to breakdown [1–3].

Nano-particles have a variety of special properties [4] because of their small sizes and large specific surface areas. In addition, nano-particles do not readily generate a 'small bridge effect' [5] even in the presence of an electric field. Therefore, the use of nano-particles to improve the performance of insulating oils has become a research topic of significant interest.

There have been many studies in which different nano-particles have been added to insulating oil to explore the effect on the performance of the oil. Du et al. [6] added nano-TiO<sub>2</sub> to oil and reported that the breakdown voltage of the oil was increased by a factor of 1.15. Katiyar et al. [7] found that a maximum breakdown voltage of approximately 68 kV was achieved when nano-scale Al<sub>2</sub>O<sub>3</sub> was

included in insulating oil at 0.25 wt.%. In addition, both nano-C<sub>60</sub> [8] and CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> (CCTO) [9] have been widely used in the study of modified insulating oils.

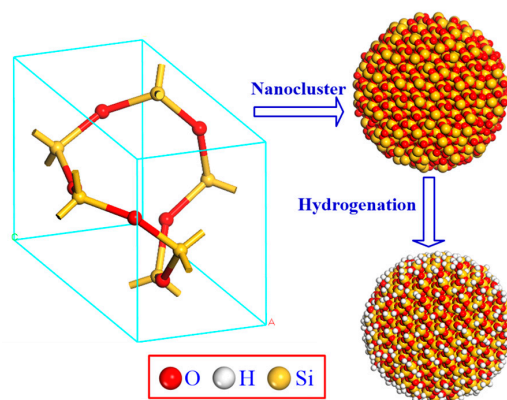
Because SiO<sub>2</sub> is an insulating semiconductor, nano-SiO<sub>2</sub> particles can mitigate the challenges associated with magnetic nano-materials that are easily affected by magnetic fields [10]. Li [11] and other researchers have also determined that the viscosity of insulating oil containing nanometer-sized SiO<sub>2</sub> particles is lowered, based on molecular simulations that assessed the effects of temperature on the viscosity of oil with nano-SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, and ZnO particles. Rafiq et al. [12] added 20% nano-SiO<sub>2</sub> particles to insulating oil and found that the AC breakdown voltage of the oil increased, although raising the humidity gradually lowered the breakdown voltage. Zhou et al. [13] combined nano-SiO<sub>2</sub> with insulating oil and showed that the breakdown voltage was considerably improved.

The above studies have demonstrated that the addition of nano-SiO<sub>2</sub> particles can effectively improve the breakdown voltage of insulating oil. However, although the presence of water is the primary cause of changes in the breakdown voltage of insulating oil, there has been little research regarding the mechanism by which nano-particles affect water diffusion in oil [14,15]. Understanding the water distribution mechanism and the effects of associated factors will therefore be an important aspect of future research regarding nano-modification. Studies have shown that, after 25 years of continuous operation, the moisture content of the average transformer is approximately 3 wt.% [16,17]. Therefore, the present work examined the diffusion behavior of water in nano-doped insulating oil in conjunction with 1 wt.%, 2 wt.% and 3 wt.% water concentrations. The diffusion behaviors associated with varying levels of water in insulating oils are discussed herein, and the mechanisms at work in nano-SiO<sub>2</sub> modified insulating oils are described on the molecular level. These results should assist in providing a theoretical foundation for further research regarding nano-modified insulating oils.

## 2. Materials and Methods

### 2.1. Model Building

A model of a cluster made of nano-SiO<sub>2</sub> particles was created using the Materials Studio 5.0 Building Tool software (version) package [18] as shown in Figure 1. After drawing the cluster, hydrogen atoms were added to the unsaturated bonds.



**Figure 1.** The model for the molecular structure of nano-SiO<sub>2</sub> particle clusters.

Mineral oil is widely used in power transformer insulation systems due to its excellent insulating properties and suitable thermal conductivity. Based on the levels of various hydrocarbons, insulating mineral oil is referred to as either paraffin or naphthenic base oil. Naphthene oil is widely used because of its excellent low temperature performance [19]. Thus, in this work, simulations were based on naphthenic mineral oil. The composition of this oil is too complex to allow all the molecular structures to be fully characterized, and so only a limited number of molecules that represent the main physical and chemical properties of the insulating oil were employed in building the model. Figure 2 shows the five alkanes used for this purpose [20], while the mass fraction of each alkane is provided in Table 1.

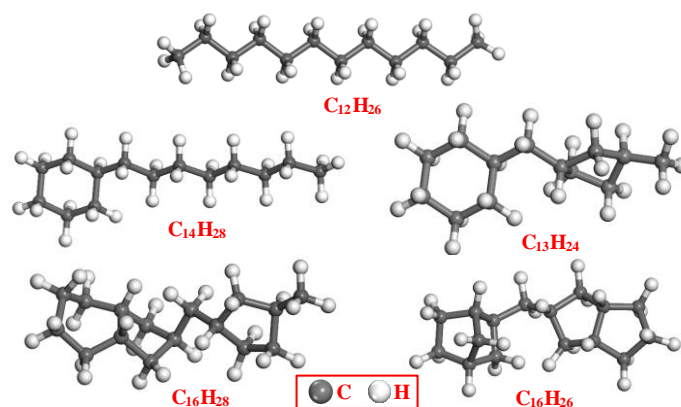


Figure 2. Molecules used during simulations of naphthenic mineral oil.

Table 1. Mass-based percentages of various molecules used during simulations of naphthenic mineral oils.

Composition	Chain Hydrocarbon	Cycloparaffins				Total
		Monocyclic	Dicyclic	Tricyclic	Tetracyclic	
$\omega_B$ (%)	11.6	15.5	28.5	23.3	9.7	88.6

Based on our goal of modeling varying levels of water in the oil, three groups of two models were constructed using Theodorou's [21] method of building amorphous polymers. Within each group, the models included an oil/water mixture containing nano-SiO<sub>2</sub> and another mixture without nano-SiO<sub>2</sub>. The mass-based percentages of water in the three groups of models were 1%, 2%, and 3%. The density of each of the six models was 0.6 g/cm<sup>3</sup> and the radius of the nano-SiO<sub>2</sub> particles was 5 Å, the concentration of the nano-SiO<sub>2</sub> particles was 5 wt.%, with a model size of 4 × 4 × 4 nm [22,23]. Figure 3 presents diagrams of the two models containing 1% water, with and without nano-particles. All MD simulations were carried out using Material Studio.

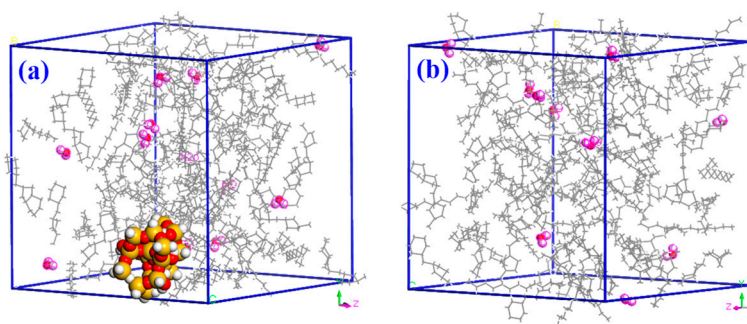


Figure 3. Diagrams of models (a) with and (b) without nano-SiO<sub>2</sub>.

## 2.2. Simulation Details

Prior to molecular dynamics simulations [24], the model was geometrically optimized, after which it was annealed and again geometrically optimized. Those systems that achieved equilibrium and energy convergence after this process could be employed for the molecular dynamics simulation. During these simulations, the model temperature was set to 70 °C [25], because this is the typical operating temperature of a transformer. Initially, the simulation was run over a time span of 200 ps at atmospheric pressure, employing a constant number of particles, pressure, and temperature (that is, an NPT ensemble), plots summarizing variations in the energy of the different models are presented in Figure 4. Subsequent simulations were performed for 300 ps using an NVT (Number of particles,

Volume, Temperature) ensemble. The integral step was set to 1 fs and the dynamic information for each atom in the system was collected at 500 fs intervals [26,27].

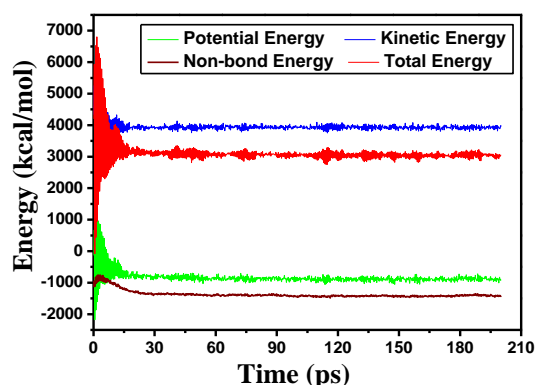


Figure 4. Variations in the energy of simulation models over time.

The COMPASS force field [28] was used during energy optimization and dynamic simulations, while the Nose and Berendsen methods were employed to control the temperature and pressure, respectively. The initial velocity of a particle was randomly assigned according to the Boltzmann distribution; the Velocity Verlet internal algorithm was used. This work also used the Amorphous Cell module to build the model, while the Forcite module was selected for model optimization and dynamic simulation.

### 3. Results

#### 3.1. Free Volume

The free volume in the model is an important factor affecting the diffusion behavior of the material, as the free volume provides the necessary active space for small particles. Thus, the size and shape of this volume affects the diffusion behavior of water molecules in the oil [29]. According to the free volume theory of Fox and Flory [30], the total volume of a polymer,  $V_T$ , is composed of the volume occupied by the polymer,  $V_0$ , and the free volume not occupied by the polymer,  $V_F$ . The ratio of free to total volume is the fractional free volume (FFV).

The free volumes of small molecules having different sizes will be different in the same model, and are primarily determined by the properties and sizes of the small molecules. This work employed the Materials Studio Atom Volume and Surface software program to create a Connolly surface, so as to calculate the free volume in the system. A hard ball probe was used, the radius of which equaled the van der Waals radius of a water molecule (1.60 Å). Figure 5 shows the Connolly surface for a two-component model with and without nano-particles, containing 1 wt.% water.

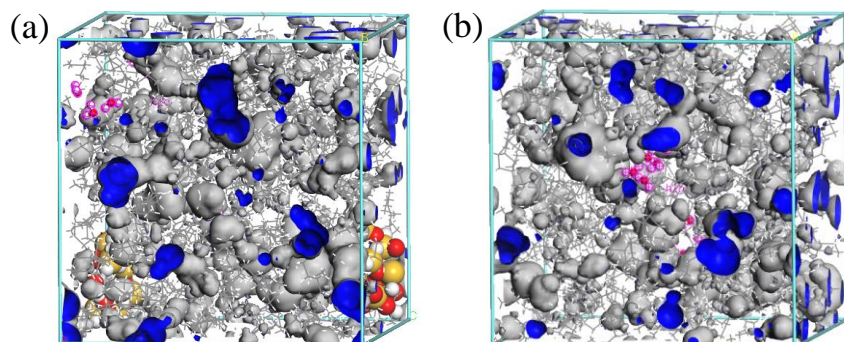


Figure 5. Free volume diagrams of the statistical Connolly surfaces for models (a) with and (b) without nano-SiO<sub>2</sub>, the blue area is the free volume and the gray area is the occupied volume.

The data in Table 2 demonstrate that the free volume fraction was smaller in those models incorporating nano-particles. In addition, increasing the water level evidently also increased the free volume fraction. These results indicate that the presence of nano-SiO<sub>2</sub> reduced the diffusion volume available to the water molecules, thus constraining the movement of water in the oil. However, with increasing water concentrations in the oil, the binding of the nano-particles to water molecules was reduced and the free volume fraction increased, allowing more free space for the diffusion of water. As a result, the difference in the free volume fractions of the models with and without nano-SiO<sub>2</sub> particles was minimized at 3% water. This result demonstrates that the effect of nano-particles on the free volume of the model decreases with increases in the level of moisture.

**Table 2.** Summarizes the free volume fractions of models having different water contents (Å<sup>3</sup>). FFV: fractional free volume.

	Nano-SiO <sub>2</sub> Particles			Without Nano-SiO <sub>2</sub> Particles		
	1%	2%	3%	1%	2%	3%
Moisture Occupied volume	35,308	35,840	34,914	34,327	34,719	33,692
Free volume	3485	3550	5902	3640	4107	5808
FFV	0.089	0.090	0.145	0.096	0.103	0.147

### 3.2. Interaction Energy

The interaction energy,  $E$ , between the water molecules and oil is also an important factor affecting the diffusion behavior of the water molecules. This value can be calculated using the Equation (1).

$$E = E_{total} - E_A - E_B, \quad (1)$$

where  $E_{total}$  is the total potential energy of the model, and  $E_A$  and  $E_B$  are the potential energy values for the oil and water molecules, respectively.

In the model containing nanoparticles, the interaction energy,  $E$  value for the water molecules and oil can be obtained from the Equation (2) [27].

$$E = (E_{total} - E_A - E_B - E_{A+C} - E_{B+C} + E_C + E_{A+B}) \div 2, \quad (2)$$

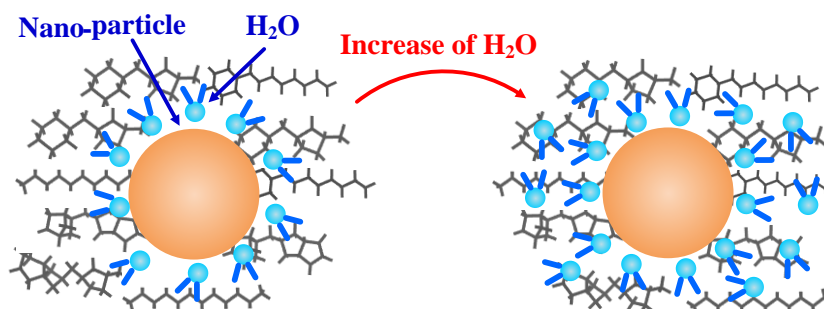
where  $E_{A+C}$ ,  $E_{B+C}$ ,  $E_C$  and  $E_{A+B}$  are the total potential energy values of the oil and nano-particles, water molecules and nano-particles, nano-particles, and water molecules and oil, respectively. Table 3 provides the interaction energy values between water molecules and oil in the six different models.

**Table 3.** The interaction energy of water molecules and oil media (kcal/mol).

	Nano-SiO <sub>2</sub> Particles			Without Nano-SiO <sub>2</sub> Particles		
	1%	2%	3%	1%	2%	3%
Moisture Interaction energy	-16.86	-30.50	-32.98	-15.80	-29.89	-30.62
van der Waals energy	-15.59	-28.24	-20.75	-14.91	-27.32	-18.75
Electrostatic energy	0.59	-0.38	-8.09	-0.578	-1.037	-10.22

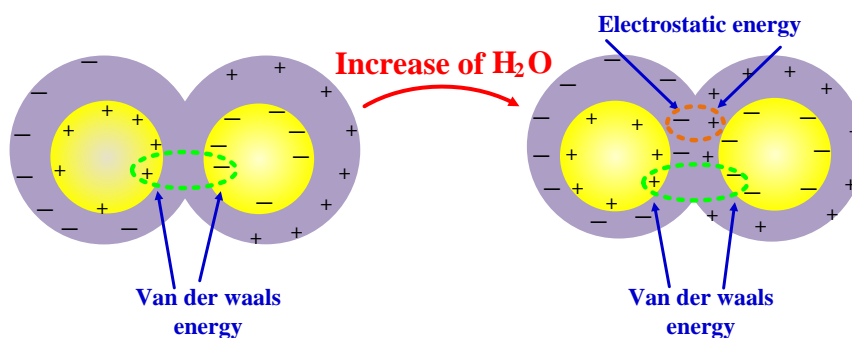
If the interaction energy is positive, the substances do not combine, whereas negative interaction energy indicates that the materials will attract one another [31]. The data in Table 3 demonstrate that, in the case of oil containing nano-particles, the absolute value of the interaction energy is larger than that of the insulating oil model without nano-particles. Therefore, the presence of nano-particles increases the binding force experienced by the water molecules. The adsorption of water molecules by nano-particles is shown schematically in Figure 6. In Figure 6 shows that nano-SiO<sub>2</sub> particles have a good effect on water molecules at low moisture content, so water molecules are evenly distributed around nano-SiO<sub>2</sub> particles. However, with the increase of water molecules, the binding of nano-SiO<sub>2</sub>

particles to water gradually weakens, so, it shows that the additional H<sub>2</sub>O is less strictly oriented in the radial direction.



**Figure 6.** The adsorption of water molecules by nano-particles.

Because water molecules and oil have very different polarities, they would not be expected to undergo electrostatic interactions, and the interaction energy is primarily due to van der Waals forces. However, in the model containing nano-particles, the electrostatic interaction energy is positive, indicating a significant change in the polarity. In the case of oil without nano-particles, the electrostatic energy is negative, suggesting that the polarity of the oil species has changed. This phenomenon further demonstrates that the nano-particles tend to adsorb water molecules, such that the water molecules do not fully interact with the oil. With increases in the water concentration, the interaction energy between the oil and water molecules increases, meaning that the oil more strongly bonds with the water. This effect is the opposite of the trend predicted by traditional free volume theory. The variations in the interaction energy with composition show that increases in the water concentration increase the polarity of the oil. As a result, there is a gradual increase in the Coulomb effect, the van der Waals forces are reduced, and the oil molecules are gradually polarized. Thus the oil molecules have a greater effect on the polar water molecules. The present research shows that the electrostatic interaction between the oil and the water molecules in the presence of nano-particles is less than that without nano-particles. This occurs because the nano-SiO<sub>2</sub> particles adsorb water such that the water in the oil has a lesser effect on the polarity of the oil. As a result, the electrostatic attraction between the oil and the water molecules is lessened. Figure 7 presents a schematic diagram that summarizes the effect of increasing the water content on the interaction energy between water and oil molecules.



**Figure 7.** A schematic summarizing the variation of the intermolecular interaction energy.

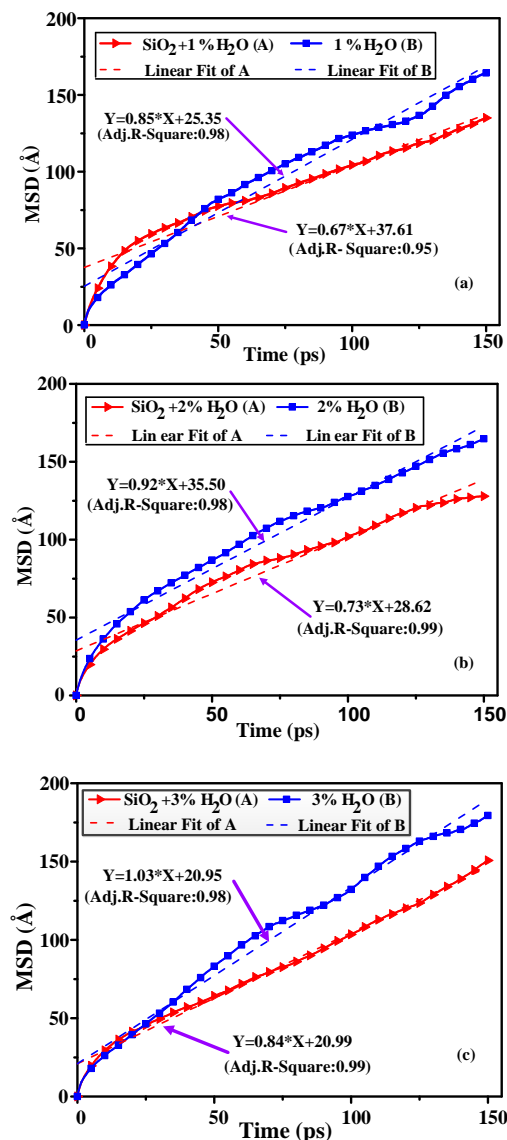
### 3.3. Mean Square Displacement

Mean square displacement (MSD) can study the diffusion behavior of water molecules in insulating oil. The diffusion coefficient is an important parameter that can be used to assess the diffusion capacity of a material. The larger the diffusion coefficient, the smaller the media's effect on

the diffusion of particles. The diffusion coefficient ( $D$ ) can be obtained from the slope of their MSD in a time interval with Einstein relation. This coefficient can be calculated via the Equation (3):

$$D = \frac{1}{6N} \lim_{t \rightarrow \infty} \frac{d}{dt} \sum_{i=1}^N (r_i(t) - r_i(0))^2, \quad (3)$$

where  $r_i(t)$  and  $r_i(0)$  are position vectors for the  $i$ th atom at time  $t$  and time zero, respectively, and  $N$  is the number of water molecules in the model. The MSD for all water molecules in each model are shown in Figure 8. To verify the Einstein relation, linear fit for all data from 0–300 ps, collect data every 2 ps. And since the beginning part of MSD is relatively chaotic, however, from the point of view of goodness of fit, it does not affect the calculation of diffusion coefficient [32].



**Figure 8.** The mean square displacement values of water molecules as functions of time for all six models (a) the mean square displacement (MSD) for water molecules of 1 wt.% moisture; (b) the MSD for water molecules of 2 wt.% moisture; (c) the MSD for water molecules of 3 wt.% moisture.

Table 4 gives the diffusion coefficients of water molecules in the various models as obtained by mean square displacement fitting.

**Table 4.** Diffusion coefficients of water molecules ( $\text{\AA}^2/\text{s}$ ).

	Nano-SiO <sub>2</sub> Particles			Without Nano-SiO <sub>2</sub> Particles		
	1%	2%	3%	1%	2%	3%
Moisture						
<i>D</i>	0.11	0.12	0.14	0.14	0.15	0.17

As can be seen from Figure 8, the correlation coefficient for each plot is greater than 0.9, showing reasonable curve fitting. The data demonstrate that, in the case of the model containing nano-SiO<sub>2</sub> particles, the diffusion coefficient is smaller than in the model without nano-particles. It shows that the diffusion ability of water molecules in insulating oil containing nanoparticles is weaker, which proves that the addition of nanoparticles can effectively restrain the diffusion of water molecules in oil. In addition, increasing the water concentration in the oil raises the diffusion coefficient of water molecules, it shows that with the increase of water content, the diffusion ability of water molecules in oil increases gradually. The classical free volume theory explains the diffusion of small molecules in amorphous polymers. The models without nano-particles show larger free volume fractions that increase with increases in the water level. This effect occurs because greater amounts of free volume provide more space for water molecules, such that the diffusion coefficient of these molecules also increases and the diffusion capacity is improved. This is in accordance with the classical free volume theory. It also provides a basis for nanoparticles to bind water molecules in oil.

#### 4. Conclusions

The diffusion behavior of water molecules in nano-modified insulating oil was studied by molecular simulations, concentrating on variations in the free volume, diffusivity and interaction energy at different water levels. On the basis of the results, we present the following conclusions.

- (1) The free volume fractions in the models containing nano-SiO<sub>2</sub> particles were reduced, and so the diffusion of water molecules was restricted. Thus, water molecules had a smaller diffusion coefficient in oils containing nano-particles, meaning less diffusion occurred.
- (2) The model containing nano-SiO<sub>2</sub> particles showed greater interaction energy between the oil and water molecules, demonstrating that the addition of these particles increased the binding of water molecules by the oil.
- (3) The results prove that the addition of nano-SiO<sub>2</sub> particles can effectively increase the binding of insulating oil to water molecules and reduce the diffusion of water molecules in insulating oil. This paper provides a theoretical basis for the modification of insulating oil with nano-SiO<sub>2</sub> particles.

**Author Contributions:** Conceptualization, W.T. and C.T.; validation, Y.Y. and S.Z.; writing—original draft preparation, W.T.; writing—review and editing, S.Z. and Q.W.; supervision, C.T.

**Funding:** This research was funded by the National Key R&D Program of China, grant number 2017YFB0902700, 2017YBF0902702.

**Acknowledgments:** The authors wish to thank the Science and Technology Project funded by the State Grid Chongqing Electric Power Co. Chongqing Electric Power Research Institute for their financial support.

**Conflicts of Interest:** The authors declare no conflict of interest.

#### References

1. Fofana, I. 50 years in the development of insulating liquids. *IEEE Electr. Insul. Mag.* **2013**, *29*, 13–25. [[CrossRef](#)]
2. Kawano, S.; Kida, T.; Miyawaki, K. Cyclodextrin polymers as highly effective adsorbents for removal and recovery of polychlorobiphenyl (PCB) contaminants in insulating oil. *Environ. Sci. Technol.* **2014**, *48*, 80–94. [[CrossRef](#)] [[PubMed](#)]



3. Zhang, S.; Chao, T.; Chen, G.; Qu, Z.; Lu, C.; Xu, L. The influence and mechanism of nano Al<sub>2</sub>O<sub>3</sub> to the thermal stability of cellulose insulation paper. *Sci. Sin.* **2015**, *45*, 1167.
4. Mansour, D.E.A.; Atiya, E.G.; Khattab, R.M.; Azmy, A.M. Effect of titania nanoparticles on the dielectric properties of transformer oil-based nanofluids. In Proceedings of the 2012 Annual Report Conference on Electrical Insulation and Dielectric Phenomena, Montreal, QC, Canada, 14–17 October 2012.
5. Xiao, B.W.; Chao, T.; Bo, H.; Jian, H.; George, C. Review of research progress on the electrical properties and modification of mineral insulating oils used in power transformers. *Energies* **2018**, *11*, 487. [[CrossRef](#)]
6. Du, Y.F.; Lv, Y.Z.; Zhou, J.Q.; Li, X.X.; Li, C.R. Breakdown properties of transformer oil-based TiO<sub>2</sub> nanofluid. In Proceedings of the Annual Report Conference on Electrical Insulation and Dielectric Phenomena, West Lafayette, IN, USA, 17–20 October 2010.
7. Katiyar, A.; Dhar, P.; Nandi, T. Effects of nanostructure permittivity and dimensions on the increased dielectric strength of nano insulating oils. *Colloids Surf. A Physicochem. Eng. Asp.* **2016**, *509*, 235–243. [[CrossRef](#)]
8. Zmarz, Y.D.; Dobry, D. Analysis of properties of aged mineral oil doped with C<sub>60</sub> fullerenes. *IEEE Trans. Dielectr. Electr. Insul.* **2014**, *21*, 1119–1126. [[CrossRef](#)]
9. Prasath, R.T.A.R.; Roy, N.K.; Mahato, S.N.; Thomas, P. Mineral oil based high permittivity CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> (CCTO) nanofluids for power transformer application. *IEEE Trans. Dielectr. Electr. Insul.* **2017**, *24*, 2344–2353. [[CrossRef](#)]
10. Cavallini, A.; Karthik, R.; Negri, F. The effect of magnetite, graphene oxide and silicone oxide nanoparticles on dielectric withstand characteristics of mineral oil. *IEEE Trans. Dielectr. Electr. Insul.* **2015**, *22*, 2592–2600. [[CrossRef](#)]
11. Yang, L.; Ming, M.; Jian, Z.D. Molecular dynamics simulation on impact of temperature on viscosity of nano-modified transformer oil. *Insul. Mater.* **2017**, *7*, 66–70.
12. Rafiq, M.; Li, C.; Lv, Y. Breakdown characteristics of transformer oil based silica nanofluids. In Proceedings of the 19th International Multi-Topic Conference (INMIC), Islamabad, Pakistan, 5–6 December 2016.
13. Zhu, J.Z.; Yi, J.; Yi, H.W. Study on characteristics of transformer oil modified by silica nanoparticles. *Insul. Material.* **2016**, *49*, 47–52.
14. Zhou, Y.; Sui, S.Y.; Li, J. Statistical analysis of moisture's effect on AC breakdown strength of TiO<sub>2</sub> nanofluids. *J. Mol. Liq.* **2018**, *249*, 420–428. [[CrossRef](#)]
15. Suleiman, A.A.; Muhamad, N.A.; Bashir, N. Effect of moisture on breakdown voltage and structure of palm based insulation oils. *IEEE Trans. Dielectr. Electr. Insul.* **2014**, *21*, 2119–2126. [[CrossRef](#)]
16. Lu, X.C.; Yu, J.; Alberto, S. Nanoparticles adsorbed at the water/oil Interface: Coverage and composition effects on structure and diffusion. *Langmuir* **2013**, *29*, 7221–7228. [[CrossRef](#)] [[PubMed](#)]
17. Xue, M.Y.; Chen, W.; Ji, Z. Influence of moisture content on electrical properties of insulating oil. *Insul. Materials.* **2016**, *7*, 79–82.
18. Xu, L.; Chao, T.; Qian, W.; Xiao, P.L.; Jian, H. Molecular simulation research on the micro effect mechanism of interfacial properties of nano SiO<sub>2</sub>/meta-aramid fiber. *Int. J. Heat Mass Transf.* **2017**, *35*, 123–129. [[CrossRef](#)]
19. Wang, X.L.; Li, Q.M.; Zhang, Y.; Yang, R.; Gao, S.G. Simulation of reactive molecular dynamics of transformer oil Pyrolysis at high temperature and the influence mechanism of acid in oil. *High Volt. Eng.* **2017**, *43*, 247–255.
20. Meng, Z.Z.; Rui, J.L.; Xin, Z. Molecular dynamics simulation of diffusion behavior for hydronium ion in hydrous oil dielectric. *High Volt. Eng.* **2011**, *37*, 1930–1936.
21. Theodorou, D.N.; Suter, U.W. Detailed molecular structure of a vinyl polymer glass. *Macromolecules* **1985**, *18*, 1467–1478. [[CrossRef](#)]
22. Zhang, S.; Tang, C.; Hao, J. Thermal stability and dielectric properties of nano-SiO<sub>2</sub>-doped cellulose. *Appl. Phys. Lett.* **2017**, *111*, 012902. [[CrossRef](#)]
23. Li, Y.; Dai, J.; Ming, D. Molecular dynamics simulation of temperature impact on the viscosity of transformer oil-based nanofluids. In Proceedings of the International Conference on Condition Monitoring and Diagnosis (CMD), Xi'an, China, 25–28 September 2016.
24. Balazs, A.C.; Zhou, Z.; Yeung, C. Behavior of amphiphilic comb copolymers in oil/water mixtures: A molecular dynamics study. *Langmuir* **1992**, *8*, 2295–2300. [[CrossRef](#)]
25. Rui, J.L.; Chun, Y.G.; Xin, Z. Diffusion behavior of gas molecules in oil-paper insulation system based on molecular dynamic simulation. *High Volt. Eng.* **2012**, *38*, 2373–2382.

26. Xiao, B.W.; Tang, C.; Wang, Q.; Li, X.; Hao, J. Selection of optimal polymerization degree and force field in the molecular dynamics simulation of insulating paper cellulose. *Energies* **2017**, *10*, 1377. [[CrossRef](#)]
27. Dai, J.Z.; Dong, M.; Wen, F.X. The Molecular dynamic simulation investigation of the dispersion stability of nano-modified transformer oil. In Proceedings of the IEEE Conference on Electrical Insulation and Dielectric Phenomena (CEIDP), Ann Arbor, MI, USA, 18–21 October 2015.
28. Song, Y.; Luo, M.; Dai, L.L. Understanding nanoparticle diffusion and exploring interfacial nanorheology using molecular dynamics simulations. *Langmuir* **2010**, *26*, 5–9. [[CrossRef](#)] [[PubMed](#)]
29. Karaborni, S.; Os, N.M.V.; Esselink, K. Molecular dynamics simulations of oil solubilization in surfactant solutions. *Langmuir* **1993**, *9*, 1175–1178. [[CrossRef](#)]
30. Fox, T.G.F., Jr.; Flory, P.J. Second-Order transition temperatures and related properties of polystyrene I influence of molecular weight. *J. Appl. Phys.* **1950**, *21*, 581–591. [[CrossRef](#)]
31. Hanus, J.; Mazeau, K. The xyloglucan-cellulose assembly at the atomic scale. *Biopolymers* **2006**, *82*, 59–73. [[CrossRef](#)] [[PubMed](#)]
32. Zhang, J.; Yu, W.; Yu, L. Molecular dynamics simulation of corrosive particle diffusion in benzimidazole inhibitor films. *Corros. Sci.* **2011**, *53*, 1331–1336. [[CrossRef](#)]



© 2018 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).