

Article

Microscopic Mechanism on the Heat Conduction of Organic Liquids: A Molecular Dynamics Study

Jing Fan, Hao Wang, Fenhong Song , Yandong Hou * and Shuangshuo Liu

School of Energy and Power Engineering, Northeast Electric Power University, Jilin 132012, China

* Correspondence: houyandong@neepu.edu.cn; Tel.: +86-13659251192

Abstract: The research on energy conversion and transportation of fuels at a microscopic level is of great significance to the development of industry. As a new alternative fuel, alcohols are widely used in industry and daily life, so it is necessary to investigate the thermophysical properties of them. In this work, seven species of pure liquid alcohols were performed to investigate the microscopic mechanisms of thermal energy transfer by non-equilibrium molecular dynamic (NEMD) method. Firstly, the thermal conductivity of alcohols was calculated and was found to be consistent with the experimental data. Then, the influence of temperature on energy transfer is investigated, the results show that the contribution of convection energy transfer increases and both the inter- and intramolecular terms decrease with the increase of temperature. Finally, the influence of molecular length on energy transfer was investigated at the same temperature, and it is concluded that the contribution of the convective term decreases and the interactive term increases to the total heat flux with increasing the length of the chain. It is worth mentioning that the contribution of intramolecular energy transfer gradually becomes a dominant part of the total energy transfer as the linear chain molecule increases to a certain length and the number of carbon atoms at the intersection point of inter- and intramolecular energy transfer is similar to the turning point of thermal conductivity.

Keywords: organic liquids; NEMD; thermal conductivity; heat conduction; molecular dynamics



Citation: Fan, J.; Wang, H.; Song, F.; Hou, Y.; Liu, S. Microscopic Mechanism on the Heat Conduction of Organic Liquids: A Molecular Dynamics Study. *Processes* **2022**, *10*, 1987. <https://doi.org/10.3390/pr10101987>

Academic Editors: Yu Liu, Ian H. Bell, Giovanni Di Nicola, Xiangyang Liu, Qibin Li and Piotr Lampart

Received: 5 September 2022

Accepted: 26 September 2022

Published: 1 October 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 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 (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

In the environment of gradual shortage of traditional fossil energy, many countries have to search new alternative fuels [1,2]. Alcohols have been widely used as an alternative fuel [3–6]. Besides, they can also be mixed with other fuels (such as gasoline, biodiesel, etc.) to enhance and improve their properties [7–11]. First and foremost, it is significant to investigate the thermophysical properties of new alternative fuels. Heat energy transfer is one of the basic issues in the physical and chemical fields. Fundamentally, it plays a significant role in revitalizing the energy industries [12]. As a basic thermophysical property, thermal conductivity is essential in optimizing the internal combustion engine and thermal design [13,14]. Experimental measurement is a common and important method to obtain the thermal conductivity of organic liquid accurately. Jin et al. [14] investigated the thermal conductivity of dimethyl carbonate using the transient hot-wire method at different temperatures from 280 to 361 K. Ogiwara et al. [15] measured the thermal conductivity of ten pure liquid alcohols and four of their binary mixtures by the relative horizontal parallel-plate method. The thermal conductivity of materials can be measured accurately and its macroscopic variation law can be obtained by experimental methods. However, the experimental method cannot capture the microscopic mechanism of heat transfer in different cases.

In recent years, molecular dynamic (MD) simulation has been increasingly emerging as the result of the rapid development of computer technology. It provides a powerful tool to analyze the heat thermal energy transfer at atomic or molecular levels [16–20] and has yielded a series of satisfactory results. Ohara [21] investigated the intermolecular energy

transfer (IET) in liquid water and its contribution by MD simulation. The results suggested that the rotational IET occupies a dominant part. Torii et al. [22] explored the contribution of inter- and intramolecular energy transfers to heat conduction in liquids of n-octane by MD simulation, and put forward a new expression to calculate the heat flux. Guevara-Carrion et al. [23] predicted the self-diffusion coefficient, shear viscosity and thermal conductivity using MD simulation and the simulated results aligned well with experimental data. Ohara et al. [24] investigated the contribution of inter- and intramolecular energy transfer of liquid n-alkanes and found that the thermal energy is mainly transferred in the space along the stiff intramolecular bonds.

Scholars have calculated thermal conductivity and investigated the energy transfer of liquid n-alkanes and alcohols. However, to the best of our knowledge, there are few studies that investigate the energy transfer of alcohols at different temperatures, and the microscopic mechanism of heat conduction of liquid alcohols is still unclear. In this paper, seven kinds of pure compound liquids of linear chain n-alcohols were selected as a representative to investigate the contribution of energy transfer in each part to the total heat flux and reveal the microscopic mechanism of heat conduction of liquid alcohols.

2. Computational Methods

2.1. Simulation System

The MD simulation system used for calculating the thermal conductivity of alcohols is shown in Figure 1. The simulation system is a rectangle cell with side lengths of 40 Å (4 ΔL , where $\Delta L = 10$ Å), 40 Å (4 ΔL) and 200 Å (20 ΔL) in an x, y, z direction, respectively. In order to eliminate the influence of the scale effect, periodic boundary conditions were imposed in three dimensional directions. The system is divided into five parts, the hot chunks with a length of ΔL are set at both ends of the system and the cold chunk with a length of 2 ΔL is set at the center of the system. The areas between the hot and cold chunks are the control volumes with a length of 8 ΔL . Furthermore, the chosen length of ΔL is larger than the structure size of n-alcohols to reduce simulation error.

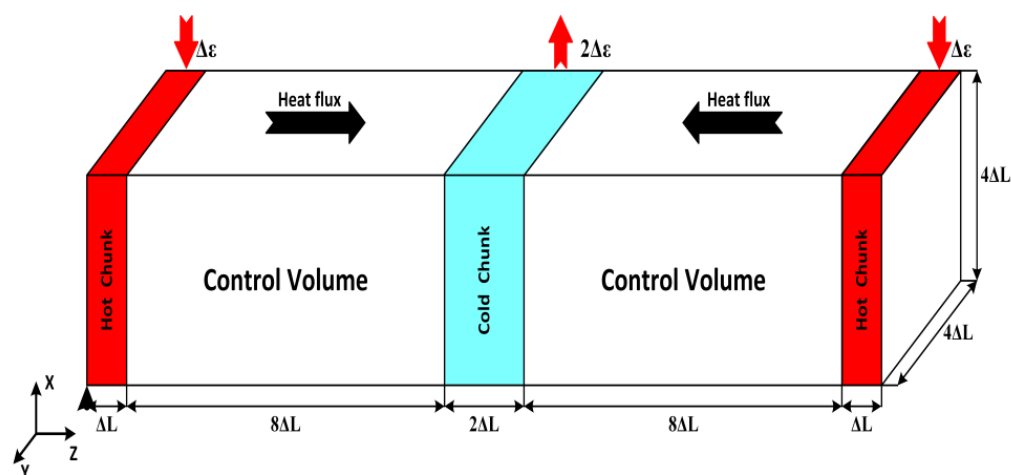


Figure 1. The simulation model for calculating the thermal conductivity of n-alcohols.

Seven kinds of n-alcohols with straight chain (i.e., C₂H₅OH, C₃H₇OH, C₄H₉OH, C₅H₁₁OH, C₆H₁₃OH, C₇H₁₅OH and C₈H₁₇OH) are selected in this paper to investigate the effect of a carbon chain on the heat transfer mechanisms. The OPLS-AA (Optimized Potentials for Liquid Simulations All-Atom) field [25,26] was applied to calculate the interactions for alcohols. The corresponding OPLS-AA calculating parameters of alcohols are generated from the LigParGen web server [27], as listed in Tables 1–4. The crossed Lennard-Jones parameters for a heterogeneous pair are obtained by the famous Lorentz-Berthelot mixed rule [28], that is, $\epsilon_{ij} = (\epsilon_i \cdot \epsilon_j)^{1/2}$ and $\sigma_{ij} = (\sigma_i + \sigma_j)/2$.

Table 1. Nonbond parameters for alcohols.

Atom Type	q (e^-)	ϵ (kcal/mol)	σ (Å)
C1(CH3-)	−0.290	0.066	3.500
C2(-CH2-)	−0.230	0.066	3.500
O	−0.590	0.170	3.120
H	0.400	0.000	0.000

Table 2. Bond stretching parameters for alcohols.

Bond Type	K_r (kcal·mol $^{-1}$ ·Å $^{-2}$)	R (Å)
CT-CT	268.000	1.529
CT-O	320.000	1.410
CT-H	340.000	1.090
O-H	553.00	0.945

Table 3. Angle bending parameters for alcohols.

Angle Type	K_θ (kcal·mol $^{-1}$ ·rad $^{-2}$)	θ (deg)
CT-CT-H	37.500	110.700
CT-CT-O	50.000	109.470
CT-O-H	55.000	108.500
CT-CT-CT	58.350	114.000
H-CT-H	33.000	107.800

Table 4. Torsion of dihedral for alcohols.

Dihedral Type	K_{Φ_1} (kJ/mol)	K_{Φ_2} (kJ/mol)	K_{Φ_3} (kJ/mol)	K_{Φ_4} (kJ/mol)
CT-CT-CT-CT	1.300	−0.200	0.200	0.000
H-CT-CT-H	0.000	0.000	0.300	0.000
CT-CT-O-H	−0.356	−0.174	0.492	0.000
CT-CT-CT-O	−1.552	0.000	0.000	0.000
H-CT-O-H	0.000	0.000	0.352	0.000
H-CT-O-H	0.000	0.000	0.352	0.000

In the system, the Verlet algorithm is used to solve Newton's equation motion with a time step of 1 fs. A cut-off radius of 15 Å is applied for calculating van der Waals interactions, and the PPPM (particle-particle particle-mesh) solver [29,30] with an accurate value of 10^{-5} is chosen for solving the Coulomb interactions to reduce computation time. Firstly, the system is equilibrated in canonical ensemble (NVT) [31,32] for 1 ns with a Nosé-Hoover thermostat and barostat to control temperature and pressure at desired values. The NVT ensemble is then unfixed and the NVE ensemble is introduced in the system to maintain energy conservation. A stable and uniform heat flux is applied to the system by using the non-equilibrium molecular dynamic (NEMD) method [33]. After running for 8 ns to reach a new dynamic equilibrium state, a temperature gradient forms in the control volumes. According to Fourier's law, the thermal conductivity can be calculated as shown in Equation (1):

$$\lambda = -\frac{J}{2tA_{xy}\langle\partial T/\partial z\rangle} \quad (1)$$

where, λ is the thermal conductivity, J is the total energy transferred in the simulation time (t) in the NVE ensemble, A_{xy} is the cross-sectional area and $\langle\partial T/\partial z\rangle$ is the temperature gradient.

2.2. Simulation Method of Heat Conduction

In the simulation system, the stable and uniform heat flux of 500 MW/m² is applied in the z-component and the heat flux [34] J_s is defined as in Equation (2):

$$J_s = \frac{1}{V_s} \left\langle \sum_{i=1} v_i e_i - S_i v_i \right\rangle \quad (2)$$

where, V_s is the volume of the system, e_i is the per-atom energy (potential and kinetic) and v_i is the velocity of atom i in the first term, and S_i in the second term is the per-atom stress tensor [35,36]. The stress tensor for atom i is given by Equation (3), where substitute x, y, z into a and b to obtain the nine components of the tensor:

$$S_{ab} = -mv_a v_b - W_{ab} \quad (3)$$

where the first term is a kinetic energy contribution for atom i , the second term is the virial contribution due to the intramolecular and intermolecular interactions and it can be approximatively expressed as Equation (4):

$$\begin{aligned} W_{ab} = & \frac{1}{2} \sum_{n=1}^{N_p} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \frac{1}{2} \sum_{n=1}^{N_b} (r_{1a} F_{1b} + r_{2a} F_{2b}) + \frac{1}{3} \sum_{n=1}^{N_a} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b}) \\ & + \frac{1}{4} \sum_{n=1}^{N_d} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) + \frac{1}{4} \sum_{n=1}^{N_i} (r_{1a} F_{1b} + r_{2a} F_{2b} + r_{3a} F_{3b} + r_{4a} F_{4b}) \\ & + Kspace(r_{ia}, F_{ib}) \end{aligned} \quad (4)$$

where, the first term is a pairwise energy contribution, r_1 and r_2 are the positions of the two atoms in the pairwise interaction, and F_1 and F_2 are the forces on the two atoms resulting from the pairwise interaction. The second term is a bond contribution of similar form for the N_b bonds which atom i belongs to. There are similar terms for N_a angles, N_d dihedrals, and N_i improper interactions. There is also a term for Kspace contribution from long-range Coulombic interaction, if defined. Furthermore, Equation (3) can be represented in the form of atomic stress [37,38]. For pairwise interactions, the atomic stress of atom i is shown as Equation (5):

$$\sigma_i^{\text{pair}} = -\frac{1}{2} \sum_{j \neq i}^N r_{ij} \otimes F_{ij} \quad (5)$$

where r_{ij} is the relative position of atom i in relation to atom j , F_{ij} is the force acting upon atom i with atom j in pairwise interaction. The sum over all the atomic stress of atoms equals the virial contribution in the system $W^{\text{pair}} = -\sum_i^N \sigma_i^{\text{pair}}$. Similarly, other terms can also be represented as this form. Hence, the stress tensor of system W^{total} can be also be expressed as follows in Equation (6):

$$W^{\text{total}} = W^{\text{pair}} + W^{\text{bond}} + W^{\text{angle}} + W^{\text{dihedral}} + W^{\text{improper}} + W^{\text{kpace}} \quad (6)$$

According to the various contributions listed above on, J_{total} can be divided into two categories, i.e., the convective term and the interaction term. The interaction term contains an intermolecular interaction term and an intramolecular interaction term:

$$J_{\text{total}} = J_{\text{convection}} + J_{\text{interact}} = J_{\text{convection}} + J_{\text{inter}} + J_{\text{intra}} \quad (7)$$

where, $J_{\text{convection}}$ includes the potential term and kinetic term, J_{inter} is composed of pairwise interaction (J_{vdW}) and Kspace interaction, and J_{intra} can be divided into bond term, angle term, dihedral term and improper term, listed as follows in Equations (8)–(10):

$$J_{\text{convection}} = J_{\text{pot}} + J_{\text{kin}} \quad (8)$$

$$J_{\text{inter}} = J_{\text{vdW}} + J_{\text{kpace}} \quad (9)$$

$$J_{\text{intra}} = J_{\text{bond}} + J_{\text{angle}} + J_{\text{dihedral}} + J_{\text{improper}} \quad (10)$$

In this study, seven kinds of n-alcohols molecules selected for simulation are all linear chain molecular, therefore, the improper energy equals zero and the improper contribution to total heat flux is zero also.

3. Results and Discussion

3.1. Thermal Conductivity

According to the NEMD method, the thermal conductivity of n-alcohols was calculated at different temperatures. To verify the simulation model and calculating method, the thermal conductivity of ethanol was investigated at temperatures $T = 233.15, 263.15, 293.15$, and 323.15 K at normal atmospheric pressure and the simulated results comparing with the experimental data [39,40] are given in Table 5 and Figure 2.

Table 5. Comparison between the simulated and experimental values of thermal conductivity for ethanol at different temperatures.

T/K	233.15	263.15	293.15	323.15
$\lambda_{\text{EXP}}/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	0.1807	0.1723	0.1650	0.1570
$\lambda_{\text{NEMD}}/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	0.1785	0.1726	0.1686	0.1590
Dev./%	−1.22	0.17	2.18	1.27

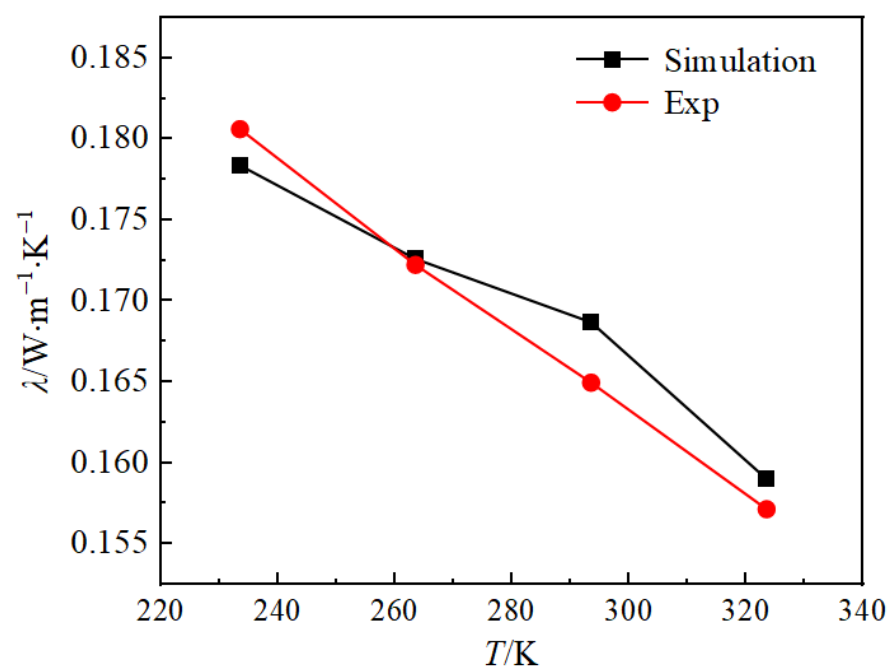
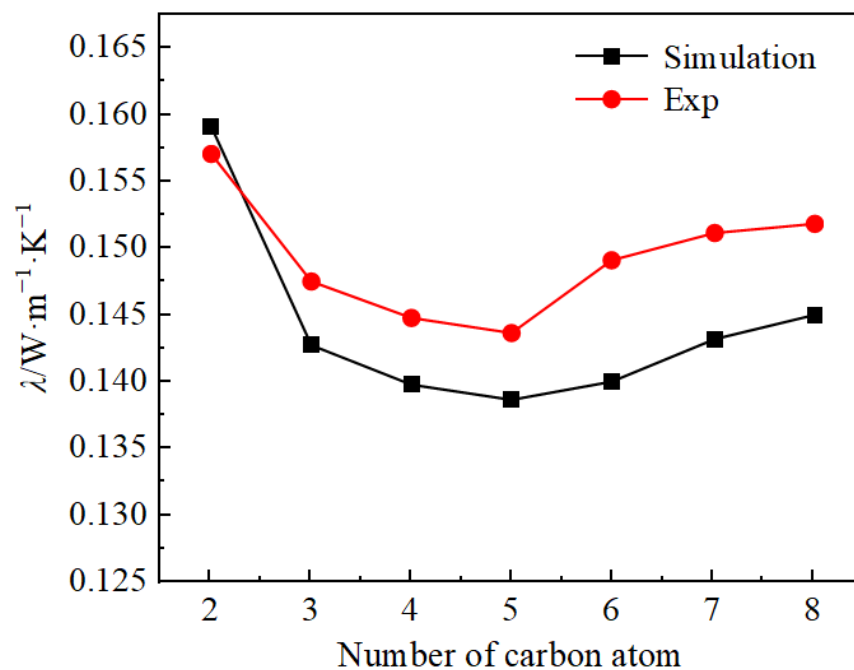


Figure 2. Comparison between the simulated and experimental values of thermal conductivity for ethanol at different temperatures.

It can be clearly seen that the thermal conductivity of ethanol decreases linearly with the increase of temperature. The relative deviation between the simulated and experimental results is less than 2.5%. Thus, the simulated values fit well with the experimental data, indicating that the simulation method and model can be applied to calculate the thermal conductivity of n-alcohols and analyze the heat transfer mechanism from a microscopic perspective. The thermal conductivity of seven kinds of liquid n-alcohols with linear chains are then calculated at a temperature of 323.15 K. The simulated results and compared experimental data are given in Table 6 and Figure 3.

Table 6. Comparison between experimental and simulated values of thermal conductivity for seven kinds of n-alcohols at 323.15 K.

Substance	$\lambda_{\text{EXP}}/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	$\lambda_{\text{NEMD}}/\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	Dev./%
Ethanol	0.1570	0.1590	1.27
1-Propanol	0.1474	0.1427	−3.19
1-Butanol	0.1447	0.1398	−3.39
1-Pentanol	0.1436	0.1385	−3.55
1-Hexanol	0.1457	0.1400	−3.91
1-Heptanol	0.1475	0.1431	−2.98
1-Octanol	0.1540	0.1449	−5.91

**Figure 3.** Comparison between experimental and simulated values of thermal conductivity for seven species of alcohols at 323.15 K.

In Figure 3, seven kinds of n-alcohols are expressed in terms of carbon atoms for convenience. It is found that the values of thermal conductivity reduce first and then increase for ethanol to 1-Octanol with the turning point at 1-Pentanol. That is, the thermal conductivity of 1-Pentanol is the smallest at the same temperature. Besides, as seen in Table 6, the maximum relative deviation is −5.91% between the simulated and experimental values [41], indicating that the simulated values are also in good agreement with the experimental values. To explore this interesting variation, several kinds of energy transfers in the n-alcohols liquids and their contributions to the total heat flux are discussed in the following sections.

3.2. Temperature Dependence of Energy Transfer

As mentioned above in Equations (8)–(10), the total heat flux of the heat transfer in organic liquid contains seven parts. In this section, ethanol ($\text{C}_2\text{H}_5\text{OH}$) was taken as an example, and the contribution of each part to the total heat flux was calculated to reveal the microscopic mechanism of heat conduction. Figure 4 depicts the contribution of each part to the total heat flux in the conduction process of $\text{C}_2\text{H}_5\text{OH}$ at different temperatures.

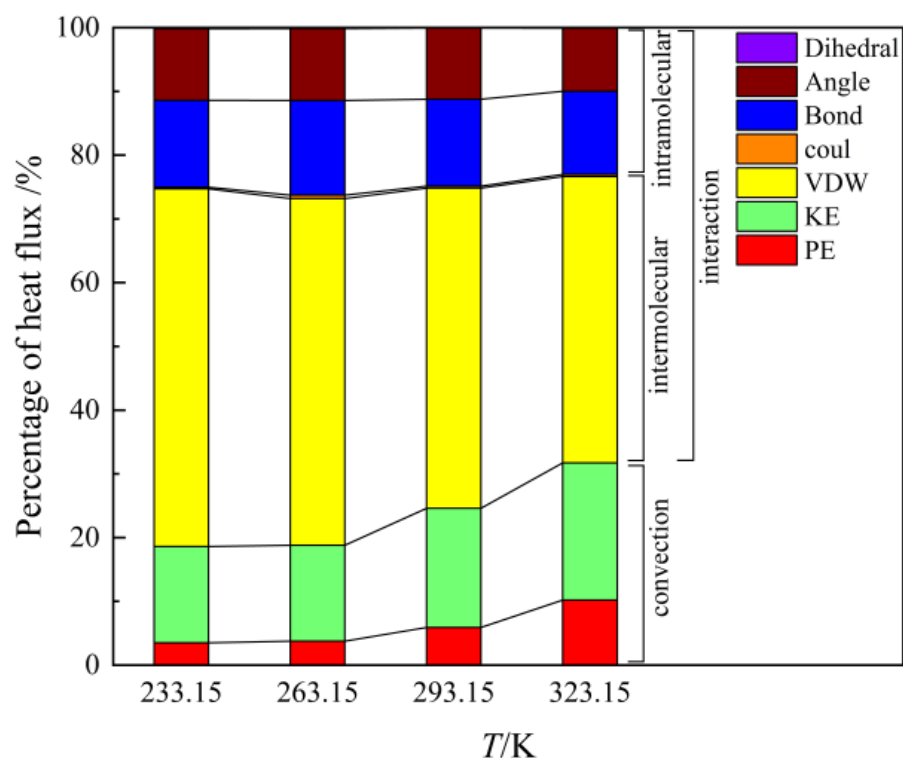


Figure 4. Contribution of each part to the total heat flux in the conduction process of C_2H_5OH at different temperatures.

It can be clearly seen from Figure 4 that the contribution of energy transfer in each part to the total heat flux changes as the temperature increases. In particular, the contributions of intermolecular and intramolecular energy transfers occupy up to 81% of the total heat flux at a temperature of 233.15 K, and it decreases to 67% of the total heat flux at a temperature of 323.15 K. Therefore, it is not hard to find out that the energy transfer of the interaction part is the dominant factor in the process of heat conduction, while, the dihedral term and Kspace term only occupies a small fraction (below 0.53%) of the total energy transfer due to the neutral molecule and little dihedral energy. To show it clearly, the contribution of these two terms are represented separately in Figure 5, and the two terms don't present a regularity with the increase of temperature. For intramolecular interaction, bond and angle interactions occupy the main part and both terms decrease with the increase of temperature. The intermolecular interaction emerges the same trend as the intramolecular term. However, the convective interaction increases as temperature increases. And in the convective interaction, the proportion of kinetic energy is larger than that of potential energy.

As the temperature increases, the thermal motion of molecules increases, resulting in an obvious increase in the contribution of energy transfer due to molecular motion. Furthermore, the total volume of liquid ethanol will increase with increasing temperature, and the density decreases in turn. The density of liquid ethanol was calculated at various temperatures and compared with the experimental data, as shown in Figure 6, and the maximum relative deviation is smaller than $\pm 3\%$ [38]. With the decrease of density, the number of molecules in per unit volume will decrease and the energy transfer efficiency will then reduce. Therefore, the thermal conductivity decreases with the increase of temperature.

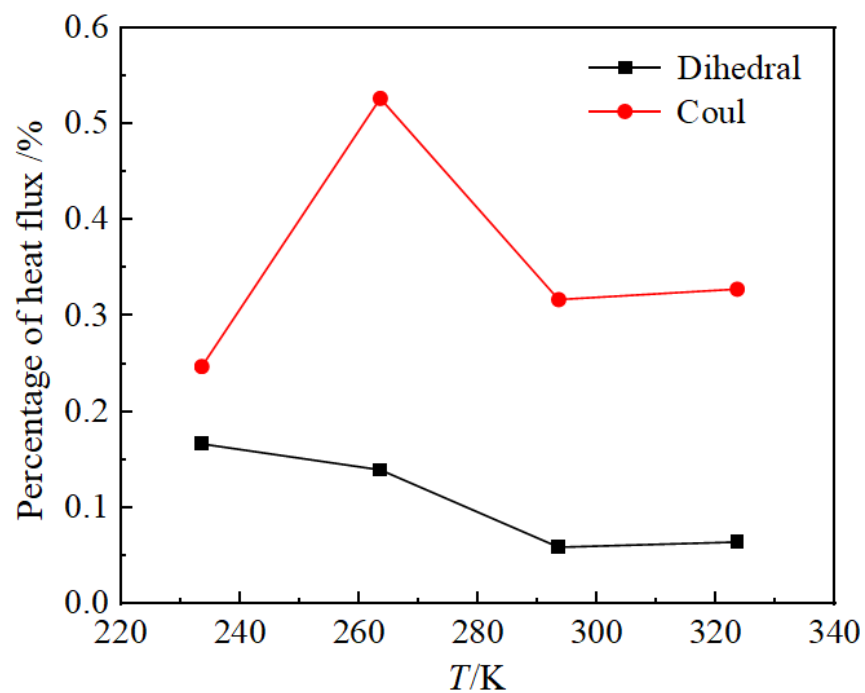


Figure 5. Contribution of energy transfer in dihedral and coul part to the total heat flux at different temperatures (C_2H_5OH).

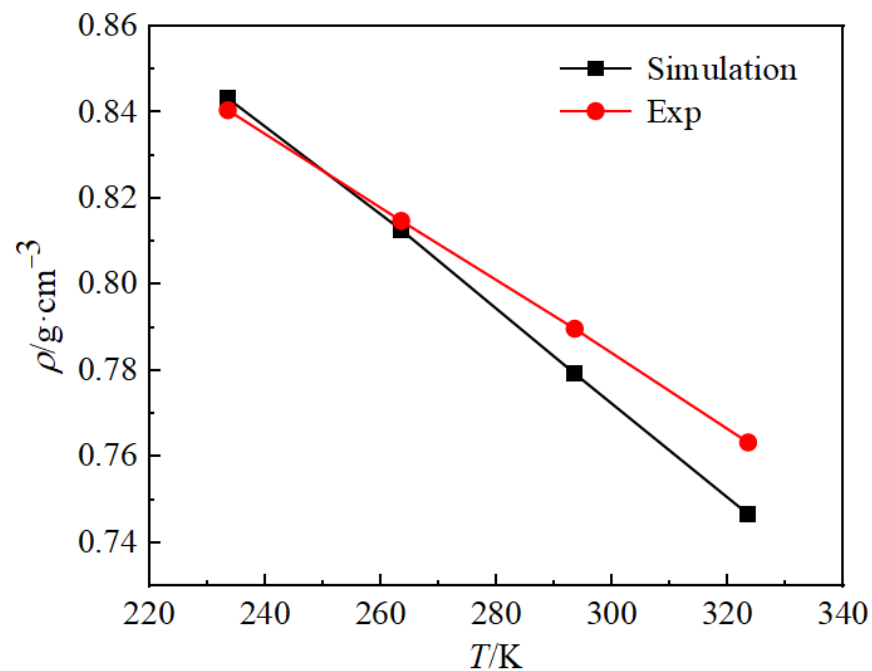


Figure 6. The simulated and experimental values of density of liquid C_2H_5OH at different temperatures.

3.3. Chain Length Dependence of Energy Transfer

For the organic liquid, molecular length affects the heat conduction because the translation, rotation, and vibration of molecular chains are related to the molecular length. The effect of molecular length on the contribution of energy transfer in each part to the total heat flux was investigated in this part. Figure 7 shows the contribution of energy transfer in each part to the total heat flux for seven species of alcohols at a temperature of 323.15 K.

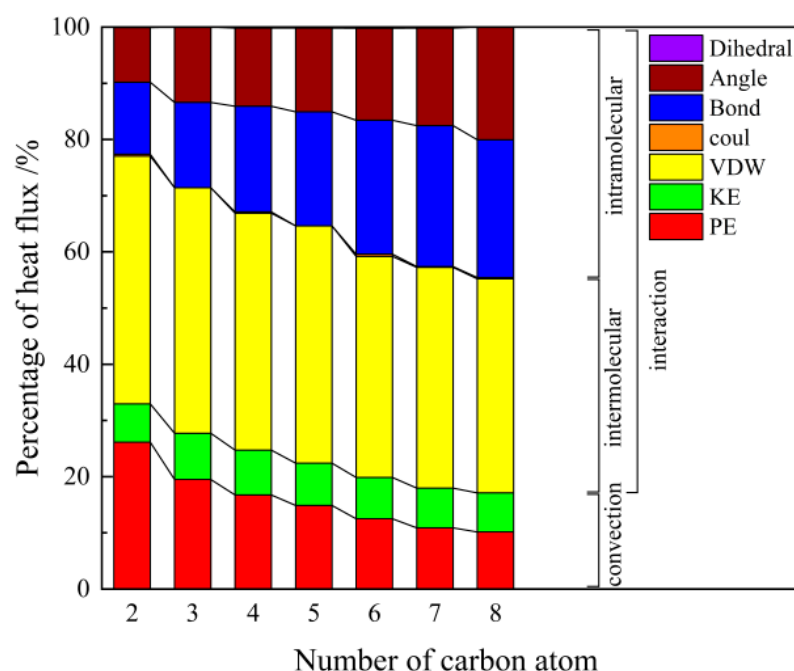


Figure 7. Contribution of energy transfer in each part to the total heat flux for seven species of alcohols at 323.15 K.

It can be seen that the contribution of interaction energy transfer to the total heat flux at 323.15 K shows an obvious increase from 67% to 83% when the number of carbon atoms increases from two (ethanol) to eight (1-Octanol). However, this increasing trend is not unlimited. Because the molecules keep moving all the time, the contribution of energy transfer due to molecular motion to the total heat flux still accounts for a certain proportion. For the interaction term, the contribution of intermolecular energy transfer occupies a dominate part in alcohols with a shorter molecular chain. By increasing the number of carbon atoms, the contribution of intramolecular energy transfer gradually increases, while the intermolecular energy transfer decreases. And the contributions of the bond and angle energy transfer occupy the most important part of the intramolecular term. The contributions of dihedral and Kspace energy transfer still account for only a small proportion (below 0.4%) because of the small amount of the dihedral energy and the neutral molecule. Similarly to that discussed above, the percentage of the dihedral term and the Kspace term shows no regularity with increasing the number of carbon atoms, as shown in Figure 8. As reported in the previous literature [34,42], the virial contribution expressed in Equation (4) might produce erroneous results in the case of heat flux when applied to systems with many-body interactions, such as angle, dihedral, or improper potentials. The contribution of angle and dihedral term is larger than what we found in this simulation. To reveal the microscopic mechanism of heat conduction very accurately, the more strict formula for calculating the heat flux with many-body interactions should be used.

It can be clearly seen from Figure 7 that the contribution of the kinetic energy transfer has hardly changed, and the potential energy transfer gradually decreases with increasing the number of carbon atoms. Through the above phenomena, it is considered that the contribution of interaction energy transfer has greater significance than the contribution of convection to the energy transfer with increasing the length of the molecular chain. In summary, the interaction energy transfer is responsible for more than 60% of the total energy transfer for seven species of liquid n-alcohols at 323.15 K, and the contribution of interaction to the total heat flux will gradually increase with increasing the length of the linear molecular chain at same temperature.

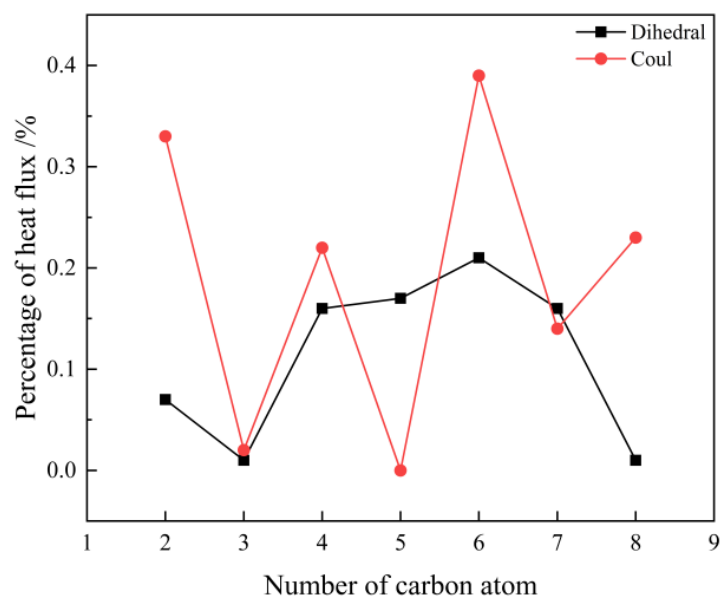


Figure 8. Contribution of energy transfer in dihedral and coul part to the total heat flux for seven species of alcohols at 323.15 K.

As the length of the linear molecular chain increases, the conversion between intermolecular and intramolecular term has aroused great interest in this work, as shown in Figure 9. This is because it might be related to the changing trend of thermal conductivity for the seven species of liquid n-alcohols (seen in Figure 3), as shown in Figure 9. It can be clearly seen that the intramolecular energy transfer increases according to increasing the length of molecules. However, this increase is gradually decelerated. The contribution of intramolecular term has reached 54% when the number of carbon atoms is eight, while the intermolecular term continues to decrease with the increase of the length of molecular chain. It is found that the number of carbon atoms at the intersection of inter- and intramolecular terms is about six, which is similar to the turning point of thermal conductivity.

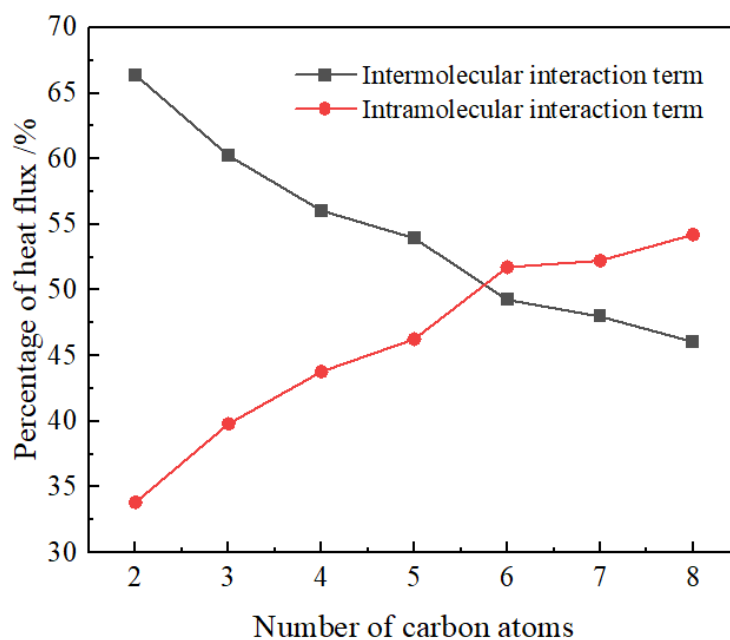


Figure 9. Ratios of intermolecular and intramolecular energy transfer to interaction term for seven species of alcohol at 323.15 K.

4. Conclusions

In this paper, a non-equilibrium molecular dynamic (NEMD) method was applied to calculate the thermal conductivity of seven kinds of liquid n-alcohols and investigate the contribution of energy transfer in each part to the total heat flux to reveal the microscopic mechanism of the heat conduction of organic liquids. Firstly, the results show that the simulated results of thermal conductivity of ethanol at different temperatures calculated through the NEMD method are consistent with the experimental data, which proves the accuracy of the simulation model and method. The effect of temperature and the length of the molecular chain on the contribution of energy transfer in each part to the total heat flux is then discussed. The results show that the contribution of interaction energy transfer dominates the process of heat conduction, even though the convective energy transfer gradually increases with the increase of temperature. With the increasing of the length of the molecular chain, the interaction term occupies up to almost 80% of the total heat flux in the conduction process, and at the same time the convective energy transfer gradually decreases. Furthermore, the inter- and intramolecular terms in the interaction part changes contrarily, and the intersection point of the inter- and intramolecular terms is similar to the turning point of thermal conductivity. According to the change of the thermal conductivity, it is obvious that intramolecular energy transfer will play an important and dominant role in the process of heat conduction if the length of the molecular chain continues to increase.

Author Contributions: J.F.: Conceptualization, Methodology, Visualization. H.W.: Software, Data curation, Writing—Original draft preparation. F.S.: Conceptualization, Software, Data curation. Y.H.: Supervision, Writing—Reviewing and Editing. S.L.: Investigation, Software. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Natural Science Foundation of Jilin Province, Grant No. 20210101088JC.

Conflicts of Interest: The authors declare that they have no conflict of interest.

References

1. Bluhm, K.; Heger, S.; Seiler, T.B.; Hallare, A.V.; Schäffer, A. Toxicological and ecotoxicological potencies of biofuels used for the transport sector—a literature review. *Energy Environ. Sci.* **2012**, *5*, 7381–7392. [CrossRef]
2. Moser, B.R. Complementary blending of meadowfoam seed oil methyl esters with biodiesel prepared from soybean and waste cooking oils to enhance fuel properties. *Energy Environ. Sci.* **2011**, *4*, 2160–2167. [CrossRef]
3. Prasad, S.; Singh, A.; Joshi, H.C. Ethanol as an alternative fuel from agricultural, industrial and urban residues. *Resour. Conserv. Recycl.* **2007**, *50*, 1–39. [CrossRef]
4. Al-Baghdadi, M. Hydrogen-ethanol blending as an alternative fuel of spark ignition engines. *Renew. Energy* **2003**, *28*, 1471–1478. [CrossRef]
5. Glaude, P.A.; René Fournet Bounaceur, R.; Molière, M. *Ethanol as an Alternative Fuel in Gas Turbines: Combustion and Oxidation Kinetics*; ASME Turbo Expo Power for Land, Sea and Air: New York, NY, USA, 2010; pp. 1–8.
6. Qian, Y.; Guo, J.; Zhang, Y.; Tao, W.; Lu, X. Combustion and emission behavior of n-propanol as partially alternative fuel in a direct injection spark ignition engine. *Appl. Thermal Eng.* **2018**, *144*, 126–136. [CrossRef]
7. Babu, D.; Anand, R. Biodiesel-diesel-alcohol blend as an alternative fuel for DIC diesel engine. *Adv. Biofuels* **2019**, 337–367. Available online: <https://www.sciencedirect.com/science/article/pii/B9780081027912000143> (accessed on 30 August 2022).
8. Awad, O.I.; Mamat, R.; Ali, O.M.; Sidik, N.; Yusaf, F.; Kadirgama, K. Alcohol and ether as alternative fuels in spark ignition engine: A review. *Renew. Sustain. Energy Rev.* **2017**, *82*, 2586–2605. [CrossRef]
9. Li, Q.; Ren, J.; Liu, Y.; Zhou, Y. Prediction of critical properties and boiling point of fluorine/chlorine-containing refrigerants. *Int. J. Refrig.* **2022**, *143*, 28–36. [CrossRef]
10. Atsonios, K.; Kougioumtzis, M.A.; Panopoulos, K.D.; Kakaras, E. Alternative thermochemical routes for aviation biofuels via alcohols synthesis: Process modeling, techno-economic assessment and comparison. *Appl. Energy* **2015**, *138*, 346–366. [CrossRef]
11. Yang, F.; Wang, X.; Tan, H.; He, S.; Liu, Z. Experimental investigations on the thermophysical properties of methyl myristate in alcoholic solutions. *Fuel* **2018**, *215*, 187–195. [CrossRef]
12. Wen, D.; Lin, G.; Vafaei, S.; Zhang, K. Review of nanofluids for heat transfer applications. *Particuology* **2009**, *7*, 141–150. [CrossRef]
13. Li, X.; Wu, J.; Liu, Z. Thermal Conductivity of liquid 2-methoxyethyl acetate, 2-ethylhexyl acetate, and diethyl succinate. *J. Chem. Eng. Data* **2012**, *57*, 2863–2868. [CrossRef]
14. Jin, X.; Wu, J.; Liu, Z.; Pan, J. The thermal conductivity of dimethyl carbonate in the liquid phase. *Fluid Phase Equilib.* **2004**, *220*, 37–40. [CrossRef]

15. Ogiwara, K.; Arai, Y.; Saito, S. Thermal conductivities of liquid alcohols and their binary mixtures. *J. Chem. Eng. Jpn.* **2006**, *15*, 335–342. [[CrossRef](#)]
16. Matsubara, H.; Kikugawa, G.; Bessho, T.; Yamashita, S.; Ohara, T. Understanding the chain length dependence of thermal conductivity of liquid alcohols at 298 K on the basis of molecular-scale energy transfer. *Fluid Phase Equilib.* **2017**, *441*, 24–32. [[CrossRef](#)]
17. Hu, J.; Liu, C.; Li, Q.; Shi, X. Molecular simulation of thermal energy storage of mixed CO₂/IRMOF-1 nanoparticle nanofluid. *Int. J. Heat Mass Transf.* **2018**, *125*, 1345–1348. [[CrossRef](#)]
18. Li, Q.; Deng, X.; Liu, Y.; Cheng, Q.; Liu, C. Gelation of waxy crude oil system with ethylene-vinyl acetate on solid surface: A molecular dynamics study. *J. Mol. Liq.* **2021**, *331*, 115816. [[CrossRef](#)]
19. Liu, X.; Zong, X.; Xue, S.; He, M. Regulating structure and flow of ionic liquid confined in nanochannel using water and electric field. *J. Mol. Liq.* **2022**, *351*, 118612. [[CrossRef](#)]
20. Liu, L.; Nicholson, D.; Bhatia, S.K. Adsorption of CH₄ and CH₄/CO₂ Mixtures in Carbon Nanotubes and Disordered Carbons: A Molecular Simulation Study. *Chem. Eng. Sci.* **2015**, *121*, 268–278. [[CrossRef](#)]
21. Ohara, T. Intermolecular energy transfer in liquid water and its contribution to heat conduction: A molecular dynamics study. *J. Chem. Phys.* **1999**, *111*, 6492. [[CrossRef](#)]
22. Torii, D.; Nakano, T.; Ohara, T. Contribution of inter- and intramolecular energy transfers to heat conduction in liquids. *J. Chem. Phys.* **2008**, *128*, 044504. [[CrossRef](#)] [[PubMed](#)]
23. Guevara-Carrion, G.; Nieto-Draghi, C.; Vrabec, J.; Hasse, H. Prediction of Transport Properties by Molecular Simulation: Methanol and Ethanol and their mixture. *J. Phys. Chem. B* **2008**, *112*, 16664–16674. [[CrossRef](#)] [[PubMed](#)]
24. Ohara, T.; Yuan, T.; Torii, D.; Kikugawa, G.; Kosugi, N. Heat conduction in chain polymer liquids: Molecular dynamics study on the contributions of inter- and intramolecular energy transfer. *J. Chem. Phys.* **2011**, *135*, 044504. [[CrossRef](#)] [[PubMed](#)]
25. Chen, B.; Martin, M.G.; Siepmann, J.I. Thermodynamic properties of the williams, OPLS-AA, and MMFF94 all-atom force fields for normal alkanes. *J. Phys. Chem. B* **1998**, *102*, 2578–2586. [[CrossRef](#)]
26. Melissa LP, P.; Dennis, O.; William, L.J. Gas-phase and liquid-state properties of esters, nitriles, and nitro compounds with the OPLS-AA force field. *J. Comput. Chem.* **2001**, *22*, 1340–1352.
27. Dodda, L.S.; Cabeza de Vaca, I.; Tirado-Rives, J.; Jorgensen, W.L. LigParGen web server: An automatic OPLS-AA parameter generator for organic ligands. *Nucl. Acids Res.* **2017**, *45*, W331–W336. [[CrossRef](#)]
28. Cui, S.T.; Siepmann, J.I.; Cochran, H.D.; Cochran, H.D.; Cummings, P.T. Intermolecular potentials and vapor-liquid phase equilibria of perfluorinated alkanes. *Fluid Phase Equilib.* **1998**, *146*, 51–61. [[CrossRef](#)]
29. Hünenberger, P.H. Optimal charge-shaping functions for the particle-particle particle-mesh (P3M) method for computing electrostatic interactions in molecular simulations. *J. Chem. Phys.* **2000**, *113*, 10464–10476. [[CrossRef](#)]
30. Brown, W.M.; Kohlmeyer, A.; Plimpton, S.J.; Tharrington, A.N. Implementing molecular dynamics on hybrid high performance computers particle-particle particle-mesh. *Comput. Phys. Commun.* **2012**, *183*, 449–459. [[CrossRef](#)]
31. Lin, Z.Z.; Liu, C.; Liu, L.; He, D.L.; Zhang, Y. Unprecedentedly High Selective Adsorption of Xe/Kr Mixtures in Carbon Nanotubes: A Molecular Simulation Study. *Chem. Eng. J.* **2020**, *393*, 124744. [[CrossRef](#)]
32. Shinoda, W.; Shiga, M.; Mikami, M. Rapid estimation of elastic constants by molecular dynamics simulation under constant stress. *Phys. Rev. B* **2004**, *69*, 134103. [[CrossRef](#)]
33. Müller-Plathe, F. A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. *J. Chem. Phys.* **1997**, *106*, 6082–6085. [[CrossRef](#)]
34. Surblys, D.; Matsubara, H.; Kikugawa, G.; Ohara, T. Application of atomic stress to compute heat flux via molecular dynamics for systems with many-body interactions. *Phys. Rev. E* **2019**, *99*, 051301. [[CrossRef](#)]
35. Thompson, A.P.; Plimpton, S.J.; Mattson, W. General formulation of pressure and stress tensor for arbitrary many-body interaction potentials under periodic boundary conditions. *J. Chem. Phys.* **2009**, *131*, 154107. [[CrossRef](#)] [[PubMed](#)]
36. Sirk, T.W.; Moore, S.; Brown, E.F. Characteristics of thermal conductivity in classical water models. *J. Chem. Phys.* **2013**, *138*, 064505. [[CrossRef](#)]
37. Egami, T.; Maeda, K.; Vitek, V. Structural defects in amorphous solids A computer simulation study. *Philos. Mag. A* **1980**, *41*, 883–901. [[CrossRef](#)]
38. Egami, T. Atomic level stresses. *Progr. Mater. Sci.* **2011**, *56*, 637–653. [[CrossRef](#)]
39. Lemmon, E.W.; Huber, M.L.; McLinden, M.O. *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1. NatlStd. Ref. Data Series*; NIST NSRDS: New York, NY, USA, 2013.
40. Chen, Q.; Wu, K.; He, C. Thermal Conductivities of [EMIM][EtSO₄], [EMIM][EtSO₄]+C₂H₅OH, [EMIM][EtSO₄]+H₂O, and [EMIM][EtSO₄]+C₂H₅OH+H₂O at T=(283.15 to 343.15) K. *J. Chem. Eng. Data* **2013**, *58*, 2058–2064. [[CrossRef](#)]
41. Fan, J.; Liu, S.; Song, F.; Wang, X. Measurements of the thermal conductivity of three pure alcohols and their binary mixtures with methyl myristate component of biodiesel. *J. Chem. Thermodyn.* **2020**, *142*, 106009. [[CrossRef](#)]
42. Boone, P.; Babaei, H.; Wilmer, C.E. Heat flux for many-body interactions: Corrections to LAMMPS. *J. Chem. Theory Comput.* **2019**, *15*, 5579–5587. [[CrossRef](#)]