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Improving the Computational Effectiveness of Molten Salt Viscosity of Alkali Metal Chlorides: A Molecular Dynamics Simulation and Theoretical Calculation Study

Jixiang Cui[1,2], *Jieting Liu*[3,*], *Mingli Zhang*[4], *Yaoqin Sun*[1,2], *Xuan Liu*[1,2], *Feiyang Han*[1,2], *Jian Xiao*[1,2] *and Haotian Liu*[1,2]

[1] Department of Power Engineering,Baoding Technical College of Electric Power,Baoding 071000, China
[2] Skill training center of State Grid Jibei Electric Power Company, Baoding 071000,China
[3] Department of New Energy Engineering, Harbin Electric Power Vocational and Technical College, Harbin 150030, China
[4] Xi’an Thermal Power Research Institute Co., Ltd., Xi’an 710054, China

SUMMARY: *Comprehensive molecular dynamic simulations were carried out to compute the viscosity and density of three commonly used chloride molten salts and their binary mixtures over a wide operating temperature range.Compared with the experimental data, the absolute relative error of the simulation results of the density and viscosity for the three kinds of chloride molten salts are all within 9.3% and 9.4%,respectively,the comprehensive results showed that the simulation results are in good agreement with the experimental values.The molecular dynamic simulations and Eyring model and molecular dynamic&theoretical caculation(MD-TC)were utilized for viscosity of binary chloride molten Salts.Compared with the experimental results,the MD-TC got more accurate results among three methods,the average error between the viscosity results of KCl-LiCl and the experimental values is only 2.03%.The results showed that it is feasible to calculate the viscosity of mixed chloride molten salts by MD-TC.In order to better understand the thermophysical properties of chloride molten salts at a molecular level, the partial radial distribution functions were calculated and local structures were analyzed. The results and methods put forth in this paper offer reference and guiding value for practical application of heat storage based on mixed chloride molten salts.*

KEYWORDS: *chloride molten salts; molecular dynamic simulations; theoretical caculation; viscosity; density*

1 Introduction

The global energy system still primarily relies on fossil fuels, including coal, oil, and natural gas, which collectively meet the majority of current energy demand. However, the combustion of these fuels leads to significant greenhouse gas emissions (GHG), contributing to climate change and global warming.According to the Statistical Review of World Energy 2023, fossil fuels accounted for approximately 82% of the world’s primary energy consumption.GHG emissions reached a record high, exceeding 40 Gt equivalent CO_2 for the first time in history [1]. Projections indicate that 2035 global energy demand will increase by nearly one-third [2]. To mitigate climate risks and align with the emissions reduction

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*ljt_hepvtc@sina.com

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targets outlined in the Paris Agreement, increasing global attention is being directed toward renewable energy sources (RES). Despite substantial progress, renewable electricity contributed only accounted for 8% of total global power generation as of 2024[1].Solar energy is widely recognized among the various RES technologies for its environmental compatibility, operational safety, and scalability [3, 4]. As a promising alternative to fossil fuels, solar energy plays a crucial role in meeting the growing energy demand of modern society.Solar power mainly includes photovoltaic (PV) and concentrated concentrating solar power(CSP) . According to data released by the National Energy Administration of By the end of 2024, China's installed solar capacity will reach 886 GW, marking an important milestone in the deployment of renewable energy [5]. However, the intermittency and volatility of solar radiation pose operational challenges for CSP systems, particularly in ensuring continuous and stable power output, thus requiring suitable thermal energy storage (TES)mediums [6]. Molten chloride salts have been used as high-temperature heat storage materials and heat transfer mediums for CSP owing to favorable thermal characteristics, such as wide operating temperature range, low vapor pressure, moderate specific heat capacity and thermal conductivity, low viscosity and cost, and high thermal stability [7, 8]. The specific heat capacity directly governs the amount of thermal energy stored, while viscosity significantly affects the system's pressure drop, pumping power, and heat transfer efficiency. Enhancing thermal conductivity is also essential for improving heat transfer performance and ensuring system safety and efficiency [9–12]. In recent years, research interest has shifted from low- to high-temperature molten salts systems, so, chloride molten salts gaining attention for their higher melting points, broad operating temperature ranges, and superior thermodynamic.[13]. However, conventional techniques for characterizing the thermophysical properties of molten salts, such as differential scanning calorimetry (DSC), are typically constrained to temperatures below 650 °C. Prolonged operation above 1200 °C can severely degrade instrument performance and accuracy [14]. To overcome these limitations, molecular dynamics (MD) simulation has become an increasingly valuable tool for investigating the thermophysical properties of high-temperature molten salts[15]. Notably, Fumi et al. [16, 17] developed a parameter set for the Born–Mayer–Huggins (BMH) potential for 17 alkali metals, which has been widely adopted in the simulation of molten salts. Building on this foundation,Ding and co-workers conducted MD simulation on pure chloride molten salts (KCl, NaCl, and LiCl) [18], as well as binary mixtures such as KCl–NaCl and KCl–LiCl [19, 20], achieving good agreement between simulated results and experimental datas for density, thermal conductivity, and viscosity.Liu et al.[21] combined experimental measurements with deep learning-assisted MD simulations to investigate the NaCl–KCl–$CaCl_2$ ternary system for high-temperature TES, reporting a high enthalpy of 251.37 J/g and prediction errors of less than 5% for both density and viscosity.Han et al.[22]synthesized $MgCl_2$–KCl–NaCl/CuO nanofluids via a solution evaporation method and found that a 0.7 wt% CuO addition increased the specific heat by 10.51% and thermal conductivity by 21.58%. Similarly,Tian et al. [23] investigated the thermal properties of SiO_2/(LiCl–KCl) nanofluids and observed that when the doping amount of SiO_2 nanoparticles is 6 wt%, the density, viscosity and thermal conductivity increase by an average of 1.22%,17.21% and 6.30%, respectively.To address the lack of high-temperature viscosity datas, Zhao et al. [24] proposed a model for predicting the viscosity of binary molten salts using only the component viscosities,densities,and mole fractions.This approach yielded a prediction error of less than 9.94%, outperforming the Eyring equation, which had an error margin of 11.4%[25]. Nevertheless, experimental data for high-temperature viscosity and density remain limited, affecting the application scope of theoretical equations.To address this gap, this study combines molecular dynamics simulation methods with theoretical calculations (MD-TC) to better predict the viscosity and density of molten salts.Compared with the experimental results and molecular dynamics simulation results, MD-TC obtained more accurate results among the three methods For instance, in the case of KCl-LiCl, the average viscosity deviation between the MD-TC method and experimental values is only 2.03%, demonstrating its strong application prospects in various temperature ranges.

2 Methodology

2.1 Force field

For molecular dynamics (MD) simulations of alkali metal-based molten salts, the Born–Mayer–Huggins (BMH) potential function is most commonly employed [26, 27]. This potential has been extensively validated and is known to describe the interionic interactions in molten salt systems accurately. Due to its effectiveness in capturing short-range repulsion and long-range Coulombic forces, the BMH potential is widely adopted in simulations involving molten salt thermophysical behavior. The functional form of the Born–Mayer–Huggins potential is expressed as:

$$U_{ij} = \frac{q_i q_j}{r_{ij}} + A_{ij}\exp\left(\frac{\sigma_{ij} - r_{ij}}{\rho}\right) - \frac{C_{ij}}{r_{ij}^6} - \frac{D_{ij}}{r_{ij}^8} \tag{1}$$

The formal charges q_i and q_i in the interaction potential are set to +1 for alkali metal cations and –1 for chloride anions, while r_{ij} represents the interatomic distance between ion centers,therefore,the first term of the potential shows the coulombic interaction. The parameter A_{ij} denotes the pauli repulsion coefficient, and σ_i & σ_j represent the ionic crystal radii of the respective ions. The parameter ρ is a hardness coefficient. Hence, the second term describes short-range repulsive forces. C_{ij} and D_{ij} are van der waals parameters for dispersion interactions.

In Table1 and 2, both the binary system parameters and corresponding pure salts parameters were listed,respectively.For binary systems such as LiCl KCl, the molar fraction of LiCl is x, and the hardness parameter ρ obeys the following rule:

$$\frac{1}{\rho_{mix}} = \frac{x}{\rho_{LiCl}} + \frac{1-x}{\rho_{KCl}} \tag{2}$$

The dispersion parameters for the Cl-Cl pair in the mixtures follow the formulas:

$$C_{mix(Cl-Cl)} = xC_{LiCl(Cl-Cl)} + (1-x)C_{KCl(Cl-Cl)} \tag{3}$$

$$D_{\mathrm{mix}(Cl-Cl)} = xD_{LiCl(Cl-Cl)} + (1-x)D_{KCl(Cl-Cl)} \tag{4}$$

Here $C_{\mathrm{Licl}(Cl-Cl)}$ and $D_{LiCl(Cl-Cl)}$ are the dispersion parameters for pure LiCl; $C_{K\mathrm{Cl}(Cl-Cl)}$ and $D_{KCl(Cl-Cl)}$ represent the corresponding values for pure KCl. The Pauli repulsion parameters A_{ij}, along with the van der Waals parameters C_{ij} and D_{ij}, are taken from references [28, 29].

Table 1: Potential parameters for the binary

	$A/KJ\cdot mol^{-1}$	σ/Å	$C/KJ\cdot mol^{-1}\cdot$ Å^6	$D/KJ\cdot mol^{-1}\cdot$ Å^6
Li-Li	42.70	1.63	4.40	1.80
Li-Cl	28.05	2.40	120.68	144.79
Li-K	32.23	2.28	80.37	51.28
Li-Na	32.23	1.99	21.14	9.04
K-K	25.45	2.93	1463.50	1445.46
K-Cl	20.39	3.05	2895.81	4404.06
K-Na	25.45	2.63	385.48	264.25
Na-Na	25.45	2.34	101.34	48.26
Na-Cl	20.39	2.76	675.68	838.59
Cl-Cl	15.28	3.17	See below	See below

Table 2: Potential parameters for pure salts system

		LiCl	KCl	NaCl
σ/Å (++)		6.82	12.26	9.79
σ/Å (+-)		10.05	12.77	11.55
σ/Å (--)		13.27	13.27	13.27
ρ/ Å		0.34	0.34	0.34
$C/ KJ\cdot mol^{-1}\cdot$ Å^6	++	4.40	1464.17	101.21
	+-	120.51	2892.21	674.84
	--	6688.24	7501.67	6989.49
$D/KJ\cdot mol^{-1}\cdot$ Å^6	++	0.13	1448.05	48.26
	+-	144.79	4404.44	838.68
	--	13454.7	12823.4	14058.0

2.2 Simulation details

All molecular dynamics simulations were performed using the open-source simulation package LAMMPS.Simulated systems include single-component molten salts (NaCl, KCl, and LiCl) and binary mixtures (LiCl–KCl and LiCl–NaCl) with molar ratios ranging from 1:9 to 9:1. Each simulation system contained 5,000 ions, arranged in a three-dimensional cubic simulation box with periodic boundary conditions to ensure bulk-like behavior and eliminate surface effects (see Figure.1). A cutoff radius of 20 Å was applied, which is less than half the box length to ensure accuracy [19]. Long-range Coulombic interactions were calculated using the Ewald summation method [30] with an accuracy threshold of $1\times10{-}4$. All simulations were conducted at an ambient pressure of 0.1 MPa. Initial atomic velocities were randomly assigned according to a Gaussian distribution. The Newtonian equations of motion were integrated using the Verlet algorithm [31] with a time step of 1 femtosecond (fs). Each simulation followed the following thermodynamic procedure:The system was first heated to 2000 K under the NVT ensemble (constant number of particles, volume, and temperature) over 100,000 time steps,Then cooled down to the target temperature over an additional 100,000 time steps under the same ensemble, Afterward,the system was equilibrated at the target temperature under the NVT ensemble for 1 nanosecond,Finally,production runs were carried out under the NPT ensemble (constant number of particles, pressure, and temperature) for 1,000,000 time steps to ensure proper relaxation.To achieve equilibrium, the temperature and pressure damping parameters were set to 100 and 500, respectively. The final results were extracted under the NVE ensemble (constant energy) over another 1,000,000 time steps, ensuring conservation of total energy. All simulations were performed on the Inspur TianShuo TS10K high-performance computing cluster, equipped with Intel Xeon E5-2620v4 CPUs (2.1 GHz, 8 cores). Each simulation was executed using 12 processor cores.

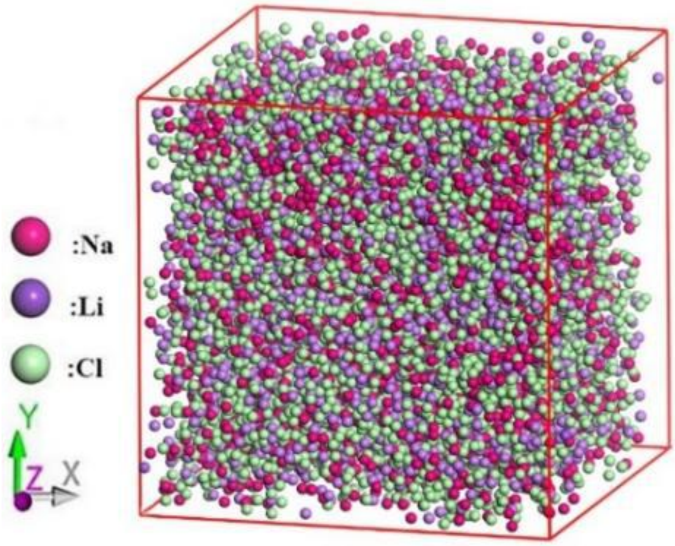

Figure 1: Simulation system of LiCl-NaCl with total number of molecules N=5000

2.3 Density Calculation

The density of the molten salts system was calculated using the following equation:

$$\rho = \frac{NM}{V_E N_A} \tag{5}$$

where:

N is the number of particles,
M is the molar mass,
N_A is Avogadro's number,
V_E is the equilibrium volume of the simulation cell obtained from the NPT ensemble at the target temperature.

2.4 Viscosity Calculation

Viscosity was computed using the Green–Kubo formalism:

$$C_p = (\frac{\partial H}{\partial T})_p \approx (\frac{\Delta H}{\Delta T})_p \tag{6}$$

The enthalpy *H* of the system was calculated as:

$$H = U + PV \tag{7}$$

where: U is the total internal energy (sum of potential and kinetic energies).

2.5 Radial Distribution Function

The radial distribution function (RDF), g(r), describes the probability of finding a particle of type β at a distance r from a reference particle of type α. It provides insights into the local structural ordering within the molten salt system. The RDF is defined as:

$$g_{\alpha\beta}(r) = \frac{1}{4\pi\rho_{\beta}r^{2}}\left[\frac{dN_{\alpha\beta}(r)}{dr}\right] \tag{8}$$

where: ρ_β is the number density of particles of type β, $N_{\alpha\beta}$ is the average number of β particles within a spherical shell of radius r centered on an α particle.

3 Theoretical Calculations

3.1 Theoretical calculation by Zhao

Zhao[24] et al. proposed a theoretical model for estimating the viscosity η of molten salt mixtures:

$$\eta_{\mathrm{e}} = \left[\eta_A[1-\left(\frac{b}{a}\right)^2\right] + \eta_B(\frac{b}{a})^2 \tag{9}$$

$$\frac{\mathrm{b}^3}{a^3} = \frac{m_B M_B / \rho_B}{m_A M_A / \rho_A + m_B M_B / \rho_B} \tag{10}$$

where, m is the molar fraction, M is the molar mass,ρ is the density.

3.2 Eyring Equation

$$\ln\eta = x_1 \ln\eta_1 + x_2 \ln\eta_2 \tag{11}$$

where, x and η are the molar fraction and viscosity of component respectively.

4 Results and Discussion

4.1 Formatting of Mathematical Components

4.1.1 Density Simulation Results of Pure Chloride Molten Salts

Figure 2 presents the simulated densities of pure chloride molten salts (NaCl, LiCl, KCl) at various temperatures.The simulated densities are slightly smaller than experimental data[32] by 9.3%, 9.2%, and 7.8% for NaCl, LiCl, KCl.These results indicate good agreement between simulation and experimental data, validating the reliability of the molecular dynamics approach for predicting the densities of binary chloride molten salts.

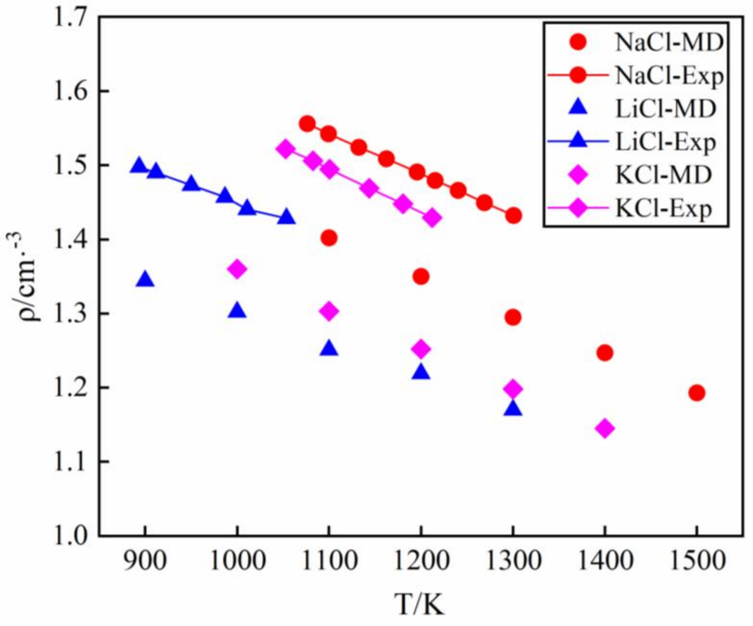

Figure 2: The density results for pure chloride molten salts with temperature

4.1.2 Density Simulation Results of binary Chloride Molten Salts

The density simulation results and experimental results of KCl-NaCl mixed in different molar ratios at different temperatures are shown in Figure 3. Compared with the existing experimental values[32], the average error is 9.8%.

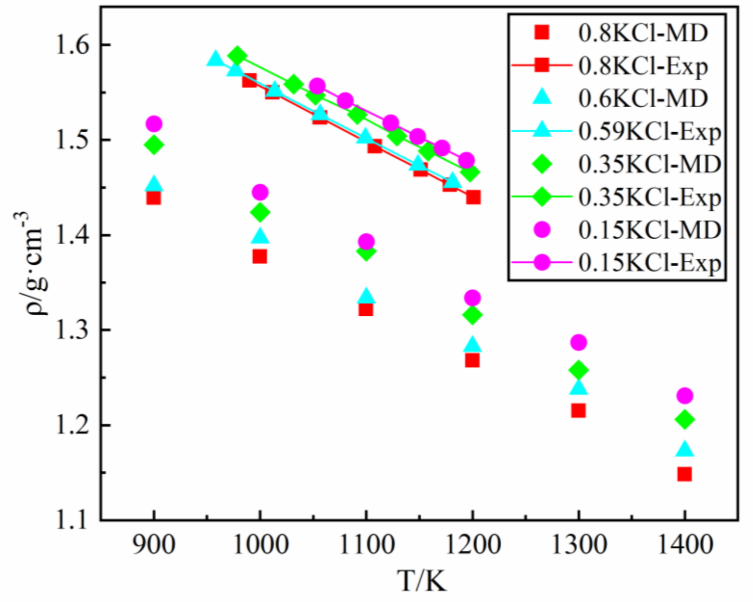

Figure 3: The density results for KCl-NaCl with temperature

The density simulation results and experimental results of KCl-LiCl mixed in different molar ratios at different temperatures are shown in Figure 4. Compared with the existing experimental values[32], the average error is 9.3%.

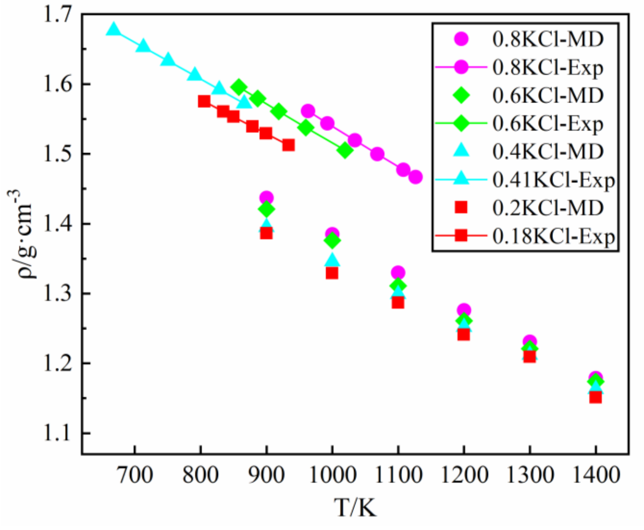

Figure 4: The density results for KCl-LiCl with temperature

4.2 Viscosity Simulation and Prediction

4.2.1 Viscosity Simulation Results of pure chloride molten salts

The viscosities of three alkali metal chloride molten salts (LiCl, NaCl, and KCl) were calculated using the Equilibrium Molecular Dynamics (EMD) method. Six independent simulations were performed for each salt to ensure statistical reliability by varying the initial atomic velocities within the system. In order to determine an appropriate correlation time for viscosity integration, the Normalized Autocorrelation Function (NACF) of the stress tensor was evaluated. Figure5(a) illustrates the decay behavior of the NACF, while the corresponding average viscosity values were computed under target temperature and pressure (or mass density) conditions. As shown in Figure5(b), compared with experimental data[33, 34], the simulated viscosities for LiCl, NaCl, and KCl exhibited average relative deviations of 9.44%, 5.15%, and 7.95%, respectively, . The relatively low error margins demonstrate strong agreement between simulation and experimental results. This also confirms the feasibility and reliability of employing molecular dynamics to predict the viscosities of binary chloride molten salts based on their single-component properties.

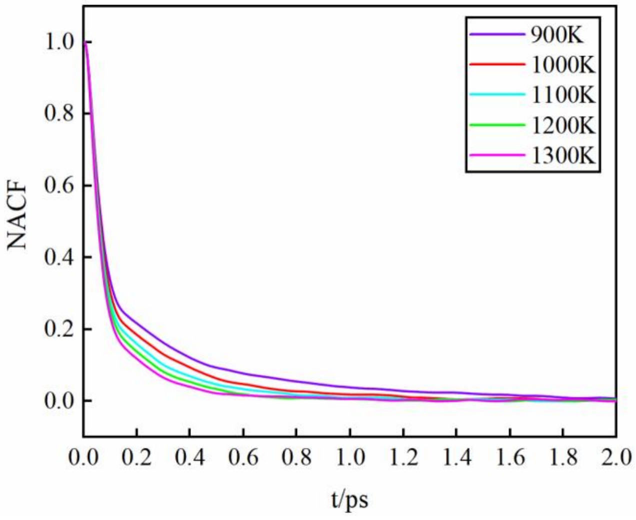

Figure 5: (a) Normalized autocorrelation function of the viscosity

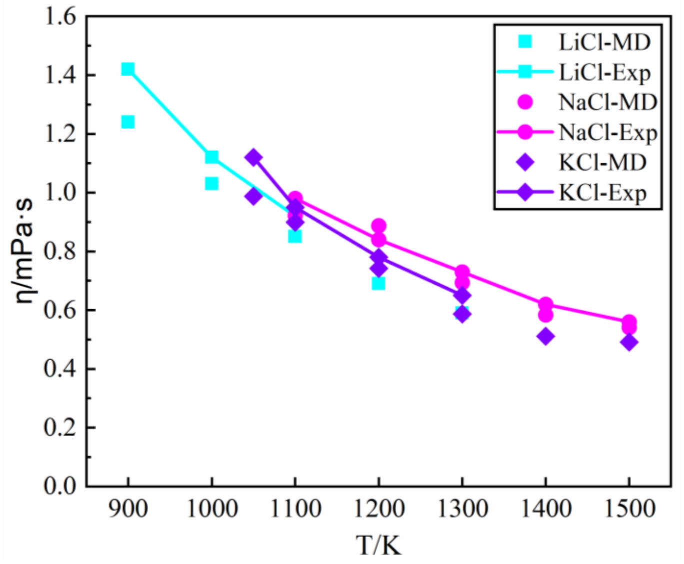

Figure 5: (b) The viscosity results for pure chloride molten salts with temperature

4.2.2 Viscosity simulation results of binary chloride molten salts

Figure 6 presents the simulated viscosities of KCl–NaCl binary mixtures at various molar ratios and temperatures in comparison with corresponding experimental data. At temperatures below 1100 K, the deviations between simulated and experimental values[35] are relatively larger. However, the discrepancies significantly decrease as the temperature increases, suggesting that the MD approach becomes more accurate under high-temperature conditions.

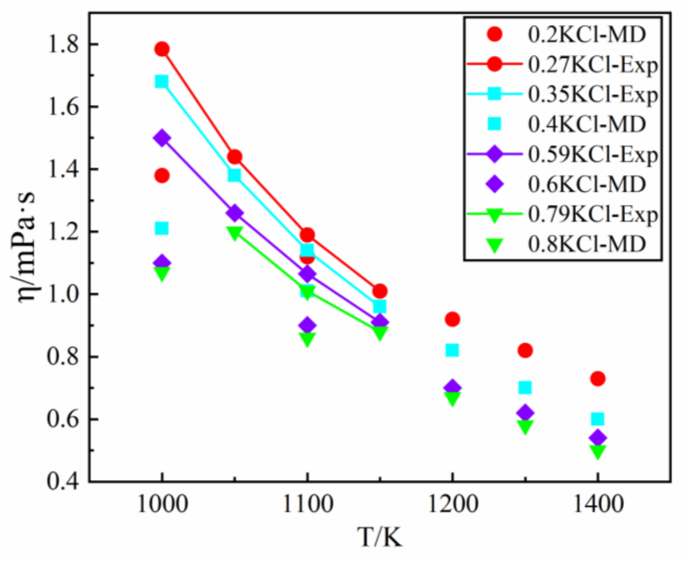

Figure 6: The viscosity results for KCl-NaCl with temperature

Figure 7 shows the viscosity simulation results for KCl–LiCl binary mixtures with different molar ratios. Across all investigated temperatures, the MD-predicted viscosities are consistently within acceptable error ranges when compared with experimental values[36], the results exhibit good agreement, further confirming the robustness of the simulation method for predicting binary molten salt viscosities.

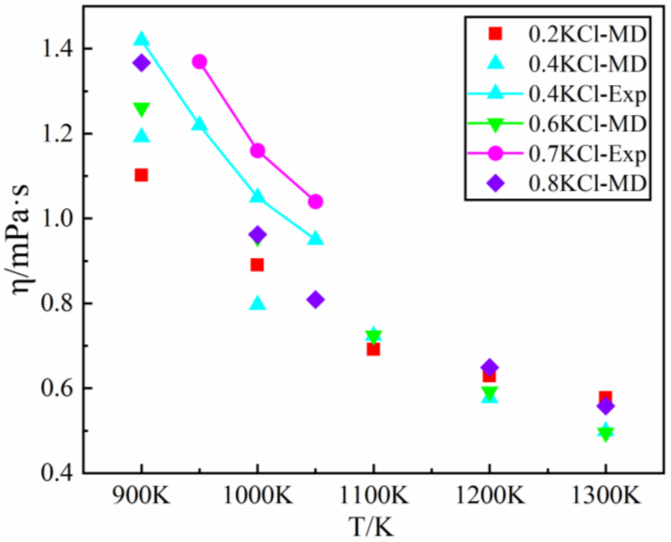

Figure 7: The viscosity results for pure KCl-LiCl with temperature

4.2.3 Theoretical Viscosity Calculation Results

The viscosities of a binary molten salt composed of 40 mol% KCl and 60 mol% LiCl were calculated using three different methods: molecular dynamics simulation, the Eyring equation, and the proposed MD–TC hybrid method. The comparison results are shown in Figure 8.The MD simulation produced an average deviation of 13.8% from experimental data. The Eyring method showed a slightly lower error of 10.3%. In contrast, the MD–TC method achieved the lowest average error of just 2.03%, indicating excellent predictive accuracy. These results suggest that integrating MD simulations with theoretical calculation frameworks offers a practical and highly accurate approach for predicting the viscosity of high-temperature chloride molten salt mixtures.

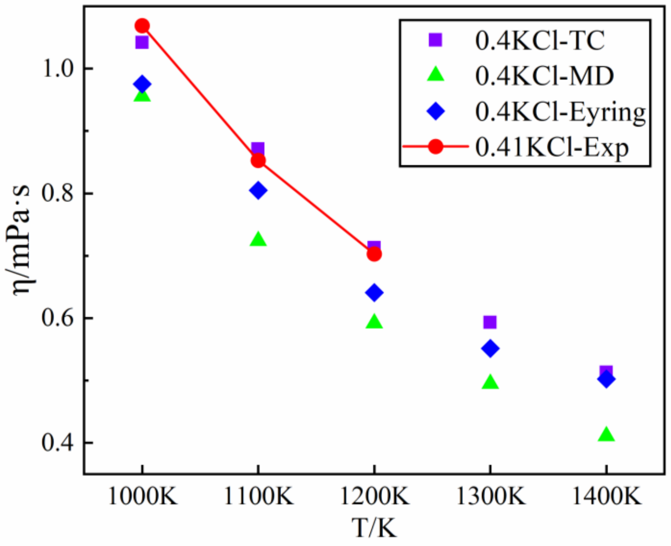

Figure 8: The viscosity results for KCl-LiCl with temperature by different methods

To further assess the reliability of the Molecular Dynamics–Theoretical Calculation (MD–TC) method, viscosity predictions were performed for a binary chloride molten salt composed of 60 mol% KCl and 40 mol% NaCl. The results, obtained via different computational approaches, are presented in Figure9. Among the methods evaluated, the MD–TC approach yielded the lowest average deviation of 9.9% compared to experimental data, outperforming standalone molecular dynamics simulations and traditional empirical models. These findings underscore the practicality of combining molecular dynamics with theoretical calculations to predict the viscosity of binary chloride molten salts. The MD–TC method enhances predictive accuracy and offers significant computational efficiency, making it a valuable tool for the thermophysical characterization of molten salt systems in high-temperature energy applications.

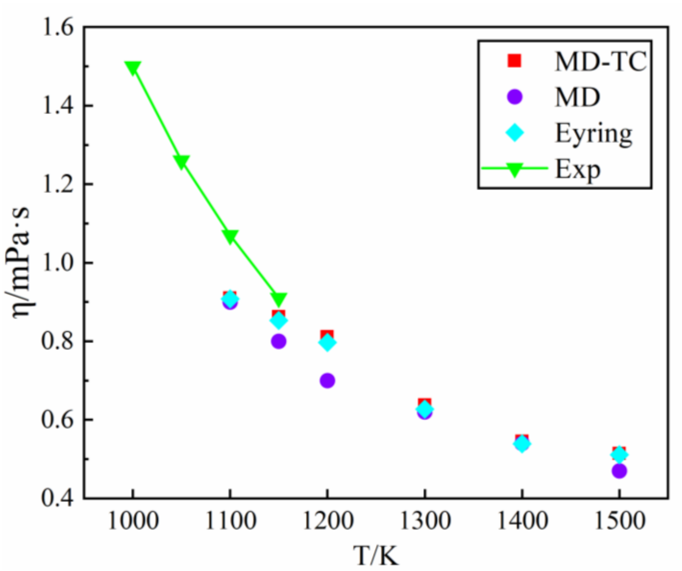

Figure 9: The viscosity results for KCl-NaCl with temperature by different methods

4.3 Radial Distribution Function Analysis

To elucidate the relationship between macroscopic thermophysical properties—specifically specific heat capacity—and temperature from a microscopic perspective, molecular dynamics simulations were employed to investigate the local structural behavior of chloride-based molten salts. The radial distribution functions (RDFs) within the cut-off radius are presented in Figure 10. The RDF, denoted as g(r), describes the probability of locating another particle at a distance r from a reference particle. It represents the ratio of the local number density of a specific particle type around a reference particle to the average number density of that particle in the entire system, thereby revealing molecular aggregation behavior and short-range structural order in liquids. The RDF is mathematically expressed as:

$$g_{\alpha\beta}(r) = \frac{1}{4\pi\pi_{\beta} r^{2}} [\frac{dN_{\alpha\beta}(r)}{dr}] \tag{12}$$

where ρ_β is the number density of species β, and $N_{\alpha\beta}$ represents the number of β particles located within a spherical shell of radius r centered on an α particle.

At temperatures above the melting point (1000–1300 K), when the chloride-based salts are in a molten state, all RDF profiles exhibit consistent features: The first peak is the highest among all peaks, indicating strong short-range ordering; The peak heights gradually diminish with increasing *r*, and converge toward a flat profile beyond the fourth weak peak at the cutoff radius, signifying short-range order and long-range disorder typical of liquid structures. In cation–anion pairs, the first RDF peak is significantly higher and narrower than subsequent peaks, reflecting strong Coulombic attraction and localized structural ordering. In contrast, the first peaks in cation–cation and anion–anion pairs are broader and less distinct from adjacent peaks, likely due to weaker electrostatic repulsion and reduced structural confinement.

As temperature increases, the height of all RDF peaks decreases, and the first peaks shift slightly to the right, indicating greater interionic distances and a more disordered structure due to enhanced ionic mobility. This structural loosening correlates with the observed reduction in viscosity at elevated temperatures for pure and binary chloride molten salts.

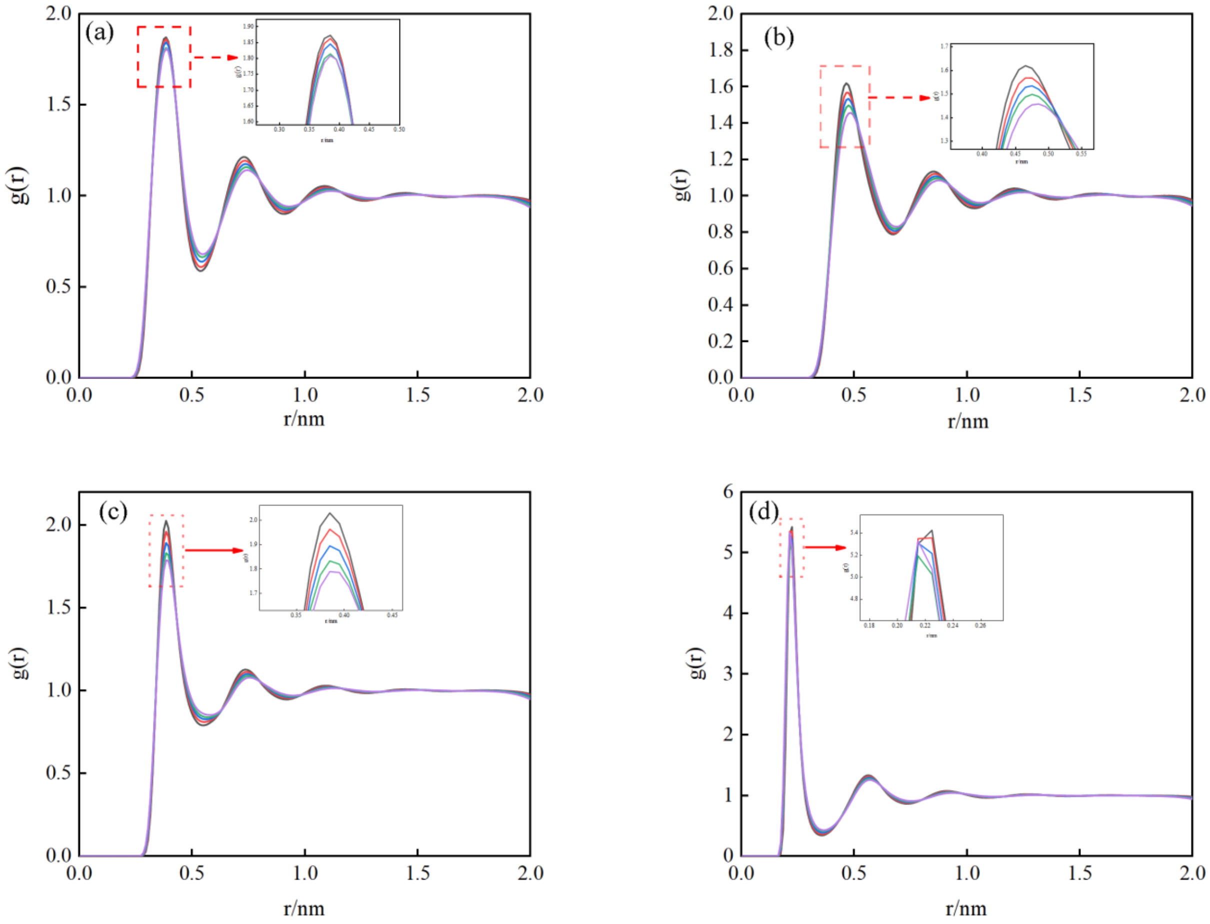

Figure 10: The partial radial distribution functions of LiCl-KCl in binary salts (a) Li-Li; (b)K-K; (c)Cl-Cl; (d)K-Cl

5 Conclusions

Molecular dynamics simulations were conducted to predict the viscosity and density of three commonly used chloride molten salts (KCl, NaCl, LiCl), and binary mixtures with varying molar ratios (LiCl–KCl, LiCl–NaCl). The simulation results for pure salts showed good agreement with experimental data, with average deviations of less than 9.4%. These findings demonstrate that MD-based methods provide a reliable reference for predicting molten salts' specific heat and related thermophysical properties.

A combined approach (MD–TC) integrating molecular dynamics with theoretical calculations was employed to predict the viscosity of binary chloride mixtures (LiCl–KCl, LiCl–NaCl). The MD-TC method exhibited superior accuracy compared with standalone MD results and the classical Eyring equation. For example, the average deviation between the MD–TC predicted viscosity of KCl–LiCl and experimental data was only 2.03%. These results confirm the feasibility of the MD–TC approach and indicate its potential for delivering more consistent and stable predictions in high-temperature molten salt systems.

Radial distribution function analysis was performed to characterize the local structural evolution of both pure and binary chloride molten salts. With increasing temperature, RDF profiles became progressively lower in amplitude, and their peaks shifted slightly outward, indicating structural relaxation. This structural trend is consistent with the observed temperature-dependent decrease in viscosity across all studied systems.

Author Contributions

Writing—original draft preparation, J.C.; supervision, Y.S. and X.L.; writing—review and editing, J.L.,M.Z and. F.H.; resources, J.X. and H.L. All authors have read and agreed to the published version of the manuscript.

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Not applicable.

Data Availability Statement

The raw data supporting the conclusions of this article will be made available by the authors on request.

Conflicts of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

About the Author

Jixiang Cui was born in Tangshan, Hebei, P.R. China, in 1995. I obtained a master's degree from North China Electric Power University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power. My main research direction is Molten salt energy storage. cjx_sgcc@sina.com

Jieting Liu was born in Hulunbuir, Inner Mongolia Autonomous Region, P.R. China, in 1997. I obtained a master's degree from North China Electric Power University in China. I am currently working at the School of Department of New Energy Engineering, Harbin Electric

Power Vocational and Technical College. My main research direction is Molten salt energy storage. ljt_hepvtc@sina.com

Mingli Zhang was born in Xi’an, Shaanxi, P. R. China, in 1993. I obtained a master's degree from North China Electric Power University in China. I am currently working at theXi’an Thermal Power Research Institute Co., Ltd. My main research direction is Transport characteristics of aviation kerosene. zhangmingli@tpri.com.cn

Yaoqin Sun was born in Baoding, Hebei, P. R. China, in 1980. I obtained a master's degree from North China Electric Power University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power.My main research direction is Molten salt energy storage. sunyaoqin@163.com

Xuan Liu was born in Baoding, Hebei, P.R. China, in 1991.I obtained a master's degree from North China Electric Power University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power.My main research direction is Molten salt energy storage. liuxuanbddy@163.com

Feiyang Han was born in Baoding, Hebei, P.R. China, in 1996.I obtained a master's degree from Tongji University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power.My main research direction is Thermal decomposition of large-sized biomass particles. hanfeiyang1996@163.com

Jian Xiao was born in Chifeng City, Inner Mongolia Autonomous Region,P.R. China, in 1982.I obtained a master's degree from Zhejiang University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power.My main research direction is Coking control of waste incineration power plants. 23505198@qq.com

Haotian Liu was born in Tangshan, Hebei, P.R. China, in 1995. I obtained a master's degree from North China Electric Power University in China.I am currently working at the School of Department of Power Engineering, Baoding Technical College of Electric Power. My main research direction is Molten salt energy storage. liuhaotian1019@126.com

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