

We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900

Open access books available

185,000

International authors and editors

200M

Downloads

Our authors are among the

154

Countries delivered to

TOP 1%

most cited scientists

12.2%

Contributors from top 500 universities



WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com



Thermal Conductivity of Dusty Plasmas through Molecular Dynamics Simulations

*Aamir Shahzad, Muhammad Qasim Khan,
Muhammad Asif Shakoori, Maogang He and Yan Feng*

Abstract

The studies of strongly coupled complex plasmas are of significant in the area of science and technology. The plasma thermal conductivity strongly coupled (complex) plasmas is of significant in scientific technology, because it behaves as complex fluids. The two-dimensional (2D) plasma thermal conductivity of strongly coupled complex dusty plasmas (SCCDPs) has been investigated by using the homogenous nonequilibrium molecular dynamics (HNEMD) simulations, proposed by Evan-Gillan scheme, at higher screening parameter κ . In our case, we have chosen particularly higher screening strength (κ) for calculating plasma thermal conductivity. The new simulations of plasma thermal conductivity are computed over an extensive range of plasma states (Γ, κ) for suitable system sizes by applying the HNEMD simulation method at constant external force field strength (F^*). It is found that the plasma thermal conductivity of SCCDPs decreases by increasing plasma states (Γ, κ). The calculations show that the kinetic energy of SCCDPs depends upon the system temperature ($1/\Gamma$) and it is independent of κ for higher screening parameter. The new results of thermal conductivity obtained from an improved HNEMD algorithm are in satisfactory agreement with earlier known numerical results and experimental data for 2D SCCDPs. It is depicted that the HNEMD method is a powerful tool to calculate an accurate plasma thermal conductivity of 2D SCCDPs.

Keywords: plasma thermal conductivity, strongly coupled, homogenous nonequilibrium molecular dynamics, force field strength, system size

1. Introduction

The thermophysical properties or physical properties of complex fluids are changed with the variation of pressure, temperature, and composition of the material, but the chemical properties remain unchanged. The phase transition of simple and complex liquids is explained by thermophysical properties [1]. Thermophysical properties consist of both thermodynamic and transport properties of fluid materials. Thermodynamic properties define the equilibrium conditions of the system which consist of temperature, heat capacity, entropy, pressure, internal energy, enthalpy and density whereas the transport properties include thermal conductivity, diffusion viscosity and waves with its instabilities. These transport properties tell

the transfer of energy and momentum to the system under consideration. The transport and thermodynamic properties contain information about the physical phenomena and help to design a system [2]. The thermal properties are calculated through experimentally, computer simulations and can predict through theoretically. The essential transport coefficient of dusty plasma is thermal conductivity and depends upon the internal energy of the particles. The thermal properties of dusty plasmas are computed for a wide combination of dusty plasma parameters by employing different computational techniques. It is a sensitive and complex parameter from the computational point of view because it directly depends on the internal energy of particles. At low temperature and high density, the thermal property of complex liquids/nonideal gases (dusty plasma) is dissimilar from ideal gases (H_2 , O_2 , N_2 , and H_2O) at same higher system parameters. For the calculation of transport properties, particular numerical models are proposed in order to investigate thermal properties for an extensive range of system temperature and density values (Γ , κ). Complex fluids (dusty plasma fluids) have used for many purposes, like power generation, semiconductors industry, cosmetics, paper industry, etc.

1.1 Significance of thermal conductivity

Thermal conductivity is the measurement of heat transfer rate in materials; the experimental parameter gives the information at the microscopic level. It has treated via theoretically based on kinetic theory, Boltzmann equation and linear response theory. The management of thermal transport is in increasing demands in the field of modern technologies. It plays a critical role in a wide variety of practical applications, such as well-organized heat dissipation in nanoelectronics and heat conduction hindering in solid-state thermoelectric. It is well established that heat transport in semiconductors and insulators efficiently modulated by materials processing or structural engineering. Though, practically all the existing approaches include altering the original atomic structure of materials that would delay due to either irreversible structure change or limited tunability of thermal conductivity. The inherent relationship between phonon behaviors and interatomic electrostatic interaction is the efficiently manipulating by thermal transport in materials fundamental thermal physical problems. Electronics cooling or high performance thermal management systems here higher thermal conductivity is needed. Phonons play a dominant role in the thermal transport of semiconductors and insulators [3]. Thermal conductivity and mass transmission over a stretched heated surface with different effects have an abundant and extensive range of applications in various engineering and industrial disciplines. These include glass blowing, extrusion process, melt-spinning, design of heat exchangers, wire and fiber coating, glass fiber production, manufacturing of plastic and rubber sheets, etc. Dusty plasma complex liquids have used in various industries such as semiconductors, energy-powered engineering industries, and microelectronics, and currently, they have vastly used in the field of nanotechnology. It is very necessary to increases thermal conductivity, which increases heat transfer rates. The main concept of the thermal conductivity of different materials and fluids is to increase the transfer heat quickly [4].

1.2 Plasma

Plasma is an ionized gas that contains neutral particles (such as molecules, radicals, and atoms) electrons and positively charged ions. In the universe, 99% of physical matter is in the plasma state and the rest part of the world is only about 1% [5]. In science and technology, plasma has extensive applications and exists in various forms. In space, most of the visible things are in the plasma state, sun and

stars are the significant examples of plasma in our universe. Constitutes of plasma show different behaviors such as quasi-neutrality that comes when positive charges and negative charges density becomes equal. Criteria of plasma at the laboratory level must satisfy three conditions by which we can say that gas is in plasma state or not at a given temperature and number of particles per centimeter cubic. These are three conditions are: (i) $N_D \gg 1$, this mathematical condition shows that the number of particles inside the Debye sphere must be greater than unity; otherwise, that particular gas at given temperature and number of particles per centimeter cubic is not a plasma. Here, $N_D = \frac{4}{3} \pi n \lambda_D^3$, where n is the number of particles, and λ_D is the Debye length. The size of the Debye length depends upon temperature and density. If the temperature is high, then the size of the Debye length will be large, and if the temperature is low, the size will be small. If the density of plasma is large, then the size of the Debye length will be small, and if the density of plasma is small, then the size of the Debye length will be large, (ii) $\lambda_D < L$, the second condition shows that the size of the ionized system must be greater than the Debye length. Here L is the size of the ionized system, (iii) $\omega_p > \nu_c$ or $T_e > 1$, the third condition shows that plasma frequency (ω_p) must be greater than the collisional frequency (ν_c), where $1/\omega_p = T_c$, here ω_p is the plasma frequency and T_c is the mean time between collisions with neutral atoms [6].

1.2.1 Types of plasmas

Plasma can be described based on different characteristics, such as density, temperature, and degree of ionization of ionized gas. Based on these characteristics, we can differentiate plasma into different types, which have succinctly discussed below. The ratio between charged particles to the total number of particles, including ions and neutrals, is proportional to the degree of ionization of plasma. The charged particle collisions dominate in plasma if the degree of ionization is high. It is low if the collisions between charged particles and neutrals have not dominated. These types are given as (i) *Cold plasma*: the number of electrons and ions equally exists in the positive column of a glow discharged tube in case of nonthermal plasmas (cold plasmas) in the laboratory. The collisions between electrons and neutral atoms depend upon the gas pressure; if the gas pressure is low, then collisions between them are not frequent, and if the pressure of the gas is high, then collisions are more frequent. The motion of gas molecules and ions have overlooked as compared to the motion of electrons because electrons have very high energy than that of the molecules of gas. That is why the nonthermal equilibrium does not exist between them. In the case of cold plasma, the temperature sequence $T_e \gg T_i \gg T_g$ exists between electrons, ions, and gas molecules. In cold plasma, only the electric forces had considered, and the magnetic effects can have ignored. The cold plasma has various applications in different fields such as medical, for example, to sterilize the surface medical instruments, meat, and meat products. For increasing the surface energy of polymers, cold plasma technology has used. To increasing printability and adhesion, the recently developed cold plasma technology has been used. (ii) *Hot plasma*: hot plasma is also known as thermal or fully ionized plasma; the collisions between ions and neutral particles are more frequently at high pressure. The temperatures of both species are approximately equal that fulfill the basic conditions of hot plasma ($T_e \equiv T_i$). In other words, we can say that in hot plasma, all the species have the same temperature. In the hot plasma, the thermal agitations of electrons, ions, and gas molecules cannot have ignored. In the case of hot plasma, the number of charges present in the cloud around the charge ball will be less than the charges on the ball. The screening is not perfect and there is the leakage of electric potential in the order of $k_B T/e$ from the cloud. This leakage of electric

potential is responsible for waves [5]. (iii) *Ultracold plasma*: the type of plasma which happens at low temperature (~ 1 K) is known as ultracold plasma and it is created in several atomic systems containing cesium, rubidium, xenon, calcium, and strontium. Any atoms that can be simply laser-cooled and has a suitable laser wavelength for photoionization have used to create ultracold plasma. The particles have strongly interacted in ultracold plasmas because their thermal energy is less than that of Coulomb energy between the adjacent particles [7]. (iv) *Ideal plasma*: the type of plasma in which Coulomb collisions are negligible, and the potential energy is minimal than the kinetic energy, then such kind of plasma is called ideal plasma. This type of plasmas has small densities and very high temperatures.

1.2.2 Role of nonideal (complex) plasma

In nonideal plasmas, the Coulomb collisions are not negligible. The mean energy of interparticle interactions increases by increasing the density. Nonideal plasmas become when the mean K.E and the mean power of the interparticle interactions become comparable. It can occur in the dense planetary atmosphere during the hypersonic motion of bodies, as a result of simulation of matter by sharp shock, concentrated laser radiations, detonation, and electric explosion waves and under the powerful chemical and nuclear explosion conditions and electron and ion fluxes. Because Coulomb collisions are active in nonideal plasmas, so, on the bases of Coulomb coupling, the nonideal (complex) plasmas have categorized in two classes. (i) Strongly coupled dusty plasma (SCDP) and (ii) weakly coupled dusty plasma (WCDP). These two terms have described by using the plasma coupling parameter Γ of a collection of charged particles, which is the ratio between potential energy to kinetic energy. Mathematically Coulomb coupling parameter is given as, $\Gamma = \langle P.E \rangle / \langle K.E \rangle \equiv Q^2 / dk_B T$. Strongly coupled plasmas, which are also known as nonideal plasmas, are the collection of a multicomponent charged particle that interacts with each other and remains at fixed positions. If the Coulomb coupling parameter “ Γ ” is more significant than unity ($\Gamma \geq 1$) then such type of plasma is called strongly coupled plasma. It is also known as cold plasma. In the laboratory, such type of plasma have generated at high density and low temperature. Due to significant interactions between neighboring dust charged particles, it has found in different phases, such as liquefy, liquid, cold liquids, and structural form. With the help of the coupling parameter structure of matter can be determined. If the Γ (Coulomb coupling) parameter is less than 1 ($\Gamma < 1$), then such type of plasma is called weakly coupled Dusty plasma (WCDP) or ideal plasma and has no structure like a gas. In weakly coupled Dusty plasmas, kinetic energy must be greater than the potential energy ($K.E > P.E$). WCDP_s has also recognized as hot plasmas, and particle motion in WCP_s is just like a molecular motion in gases. In hot plasma, thermal agitations are present, and screening will not be perfect.

1.3 Complex (dusty) plasma and applications

Plasma consists of electrons, ions, and neutral atoms; in addition to dust particles is known as dusty (complex) plasma. Due to dust particles, the physical properties of the plasma become complicated; that is why we call them also complex plasma. The study of dusty plasmas has become a developing branch of plasma physics in the field of sciences, technologies, and space. The study of dusty plasmas had become interesting for research of laboratory plasma when the formation of dust and dust trapping was observed during the plasma etching of silicon wafers and to limit the deposition rate when powder formation in plasma-enhanced CVD was identified. Dust is present everywhere in the space, such as interplanetary dust

in planetary rings and in comet tails, and also it have present in the atmosphere and earth magnetosphere. These charged particles interact with each other and with the plasma constituents such as electrons, ions, and neutral atoms due to which plasma behavior becomes complicated [8]. These charged dust particles change the properties of plasma by electric and magnetic fields. The value of the Coulomb coupling parameter between dust particles is high due to the massive dust charge, which leads to the liquid and solid phase of the dust system at room temperature. For study the phase transitions and structural properties of solids, Yukawa balls and plasma crystals are appropriate systems. Plasma with dust particles can be termed as either “dust in plasma” or “dusty plasma” depending on the ordering of several characteristic lengths and radius between interacting particles (r_d and λ_D). If the Debye length of dust particles (λ_{Dd}) is less than the interparticle distance (r_d) then it is called dust in plasma. Mathematically it is written as $\lambda_{Dd} < r$. Here “ r_d ” is the interparticle distance, and “ λ_{Dd} ” is the Debye length of dust particles. In this case, there are no dust particles in the plasma sphere. If the Debye length of dust particles (λ_{Dd}) is greater than the interparticle distance (r) then it is called dusty plasma. Mathematically it is written as $\lambda_{Dd} > r$ and it shows that dust particles are present in the plasma sphere.

In industrial applications, dust particles distributed in the plasma and produced disturbing effects in plasma. This contamination in the plasma has devastating effects on the fabricated circuits. On the other side, applications such as surface processing make the use of dust particles that have spread in the plasma. For example, the growth of carbon-based nanostructures on the surface used for electronic devices such as sensors, silicon-based films which have used in solar cells, and flat-panel displays illustrates an enhanced performance of nanoparticles produced in the plasma through chemical reactions, are inserted into the film. Through plasma processing, the coating of particles has produced. Plasma-based materials processing technologies have widely used in the manufacturing of integrated circuits. To etch, sputter, or modify the surface properties of silicon wafer, chemically reactive plasma have used. The fine dust particles created in plasma chemical systems have useful and exciting features that also control their compositions and size. It has used to grow or modify existing materials.

1.3.1 Merits and demerits of dust particles

Initially, the dust has not considered a useful technological consequence in the plasma. It has simply considered an unwanted pollutant in the plasma. To minimize the negative influences of dust particles in the plasma leads to the development of material science. The nanoparticles have considered as the basic building blocks of nanotechnology in plasma discharges. There are many advantages of dust particles in dusty plasmas such that nanocrystalline silicon particles have used to enhance the lifetime and efficiency of silicon solar cells, which have developed in silane plasmas. Dust particles have used to improve the surface properties of materials by applying plasma-enhanced CVD systems. The thin films produced by PECVD systems of TiN in an amorphous Si_3N_4 matrix have very high elastic modulus and hardness. In hydrocarbon plasmas such as methane or acetylene, carbon-based nanostructures have developed to govern thin carbon films, which lead to materials of high hardness, wear-resistance, and chemical inertness. In Ar/CH_4 plasmas, the fabrication of nanocrystalline diamond films has done. These films have unique properties such as high hardness, chemical inertness, and extreme smoothness [9]. Dust particles are also used in the ceramic industry for sintering and in the fabrication of hard coatings, and also used in optical devices. Dust particles decrease the performance and the yield of many electronic devices. In the semiconductor industry, dust

particles reduced the performance and yield of semiconductors. Dust particle contamination in the medical field during the production of different kinds of medicines has serious issues. The dust particles are of micron-sized, which reduces the adhesion of thin films of different materials due to deposition on the surfaces and also creates dislocations. In industrial applications, dust particles contamination in the plasma creates many defects in the manufacturing of microchips and fabricated circuits. Dust particles disturb the stability and the safety of the plasma in fusion reactors.

2. Molecular dynamics simulations

Over the last seven decades, the computer performance's speed to elementary calculations has increased by 10^{15} factor. The computer memories, data storage also increased at a similar speed. Nowadays, by using computer simulation, we can save both time and money. The fundamental purpose of computer simulation is to guide the real experiment more precisely. Computer simulations used to predict various properties of gases, liquids, solids, and biological organisms. It is very useful for checking theoretical results, understanding experimental observation for the case where no academic data available. It also allows us to the identification of essential processes and visualization of the system [10]. The molecular dynamics simulations (MDS) one of the computer simulations techniques, in these technique atoms and molecules, are assumed to follow Newton's law as $F_i = ma_i \equiv m d^2 r / dt^2$, where F , m and a represent the force, mass, and accretions of i th particles in x -coordinate direction. In this book chapter, we integrate this equation by the predictor-corrector method. MDS has two basic types depends on the properties, which we are going to calculate one is equilibrium molecular dynamics simulations (EMDS), and another is nonequilibrium MDS (NEMDS). In this work, we have applied NEMDS to investigate the thermal conductivity of SCDPs at different dusty plasma parameters [11, 12].

2.1 Numerical model and algorithm

NEMDS is used to obtain the trajectory of dust particles' motion of a system [13] that interacts with each other through an interparticle Yukawa potential [14]. Homogeneous nonequilibrium molecular dynamic simulation (HNEMDS) approach have used for the calculation of thermal conductivity of complex (dusty) plasma liquids, which are molded, using a most common Yukawa (screened Coulomb) potential for charged particles [15] and has the following form,

$$\phi_Y(|\mathbf{r}|) = \frac{Q^2}{4\pi\epsilon_0} \cdot \frac{e^{-|\mathbf{r}|/\lambda_D}}{|\mathbf{r}|} \quad (1)$$

Here " r " is the magnitude of interparticle distance, Q is the charge of dust particles, and λ_D is the Debye screening length. We have three normalized (dimensionless) parameters to characterize the Yukawa interaction model $\phi_Y(|\mathbf{r}|)$: (i) the plasma Coulomb coupling parameter define as: $\Gamma = (Q^2/4\pi\epsilon_0) \cdot (1/a_{ws}k_B T)$, where a_{ws} is Wigner Seitz radius and it is equal to $(n\pi)^{-1/2}$, here n is the number of particles per unit area (N/V). The k_B and T are Boltzmann constant and absolute temperature of the system, (ii) the screening strength (dimensionless inverse) $\kappa = a_{ws}/\lambda_D$, and (iii) normalized external force field strength, $F^* = (F_Z) \cdot (a_{ws}/J_Q)$ [15, 16]. We have applied periodic boundary conditions and Gaussian thermostat in

canonical ensemble (NVT) in order to constant temperature for a Yukawa system. The further detail of these three dimensionless parameters is given in our earlier work of Refs. [15–17]. We started from a well-known, the Green-Kubo relations (GKR_S) for the hydrodynamic transport coefficients of uncharged particles [18]. This important GKR_S of pure liquids have applied to calculate the thermal conductivity of 2D and 3D SCCDP_S [11, 12, 19–27].

$$\lambda = \frac{1}{2k_B A T^2} \int_0^\infty \langle \mathbf{J}_Q(t) \cdot \mathbf{J}_Q(0) \rangle dt, \quad (2)$$

where in Eq. (2), k_B is the Boltzmann's constant, A is the system area, T is the system temperature, and \mathbf{J}_Q is the current heat vector at time t of 2D case. In our MD simulation, the angular brackets represent an ensemble average. In this model, the expression for the microscopic heat current vector \mathbf{J}_Q [16, 17] can be given by

$$\mathbf{J}_Q(t)A = \sum_{i=1}^N E_i \frac{\mathbf{p}_i}{m} - \frac{1}{2} \sum_{i \neq j} (\mathbf{r}_i - \mathbf{r}_j) \cdot \left(\frac{\mathbf{p}_i}{m} \cdot \mathbf{F}_{ij} \right) \quad (3)$$

Where \mathbf{F}_{ij} is the total interparticle force at time t , on particle i due to j , $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ are the position vectors (interparticle separation), and \mathbf{P}_i is the momentum vector of the i th particle. Where, E_i is the total energy of particle i , and is given by the expression as

$$E_i = \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \phi_{ij} \quad (4)$$

Where ϕ_{ij} is the Yukawa pair potential between particle i and j and given by Eq. (1). Here, in Eq. (4) the first term represents the kinetic energy (K.E), and the second term represents the potential energy (P.E). The Evan's [28–30] proposed the non-Hamiltonian linear response theory (LRT), has been used for a moving system representing the equation of motion

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m} \quad (5)$$

$$\dot{\mathbf{p}}_i = \sum_{j=1}^N \mathbf{F}_i + \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i) \cdot \mathbf{F}_e(t) - \alpha \mathbf{p}_i \quad (6)$$

In Eq. (6), $\mathbf{F}_i = (-\partial\phi_{ij}/\partial\mathbf{r}_i)$ is the total Yukawa interparticle force acting on particle i in an N -particle system and $\mathbf{D}_i = \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i)$ is the phase space distribution function with \mathbf{r}_i and \mathbf{p}_i being the coordinate and momentum vectors of the i th particle. Mechanical work is performed through the externally applied force field $\mathbf{F}_e(t)$ and thus the equilibrium cannot be maintained. In the above expression, α is the Gaussian thermostat multiplier that keeps the system temperature [15–22, 28] and it is given as

$$\alpha = \frac{\sum_{i=1}^N [\mathbf{F}_i + \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i) \cdot \mathbf{F}_e(t)] \cdot \mathbf{p}_i}{\sum_{i=1}^N p_i^2 / m_i} \quad (7)$$

When an external force field parallel to the z -axis is of the form $\mathbf{F}_e(t) = (0, F_z)$, in the limit $t \rightarrow \infty$ [15, 31] then, the thermal conductivity is calculated as

$$\lambda = \frac{1}{2k_B A T^2} \int_0^\infty \langle \mathbf{J}_{Q_z}(t) \mathbf{J}_{Q_z}(0) \rangle dt = \lim_{F_z \rightarrow 0} \lim_{t \rightarrow \infty} \frac{-\langle \mathbf{J}_{Q_z}(t) \rangle}{TF_z} \quad (8)$$

In Eq. (8), $\mathbf{J}_{Q_z}(t)$ is the z-component of the current heat vector and the external force field $\mathbf{F}_e(t) = (F_z)$ [15–22, 31].

In this study we have used the same method as employed in our earlier work of 3D strongly coupled dusty plasmas [11, 12]. The most computational time consuming part of used algorithm is to compute the interparticle interactions (force and internal energy). It has been shown in our previous work that the proposed method has advantage to calculate Yukawa forces and relevant energy in appropriate computational time with reasonable computational power. In our present case, the HNEMD method is used to compute the thermal conductivity of 2D plasma systems and production stage of thermal conductivity is obtained between $10^6/\omega_p$ and $2 \times 10^6/\omega_p$ time units for each plasma states. It shows that the used method is computational time cost-effective and power saving as compared to earlier methods based on different numerical schemes [12, 14, 26, 27].

3. Simulation results and discussion

In this section, the processing of the data of our computer simulation gave us the numerical results of the thermal conductivity of 2D complex (dusty) plasmas. We have used HNEMD simulations over the wide range of plasma Coulomb Couplings Γ ($=10, 500$) and four higher Debye screening strengths κ ($= 4.5, 5.0, 5.5$, and 6) at constant low normalized external force field strength F^* ($=0.02$). In the present work, our 2D SCDPs through HNEMD simulations have carried out for a constant number of particles ($N = 400$) in a simulation box with edges length (L_x, L_y). We have applied to the squared simulation box wraparound periodic boundary conditions (PBC). For nonequilibrium conditions of the systems, we run our MDS code 200000 time steps. Here we have used constant $dt = 0.001$ in integrated equation via predictor-corrector algorithm for the calculations of dust particles positions, velocity and acceleration. For each time step, the position, velocity, acceleration and forces of each spherical dust particles are calculated and update it. The HNEMD method is more powerful for computing forces and energy of Yukawa interactions and more effective as compared to earlier numerical methods of 2D and 3D ([13, 14, 23–27] and their references herein).

Figures 1 and **2** present the simulation results obtained by applying the Evan-Gillan HNEMD approach of thermal conductivity (λ_0) with appropriate normalization (plasma frequency, ω_p) as $\lambda_0 = \lambda/nm\omega_p a^2$, at the normalized external constant force field strength F^* (0.002) for 2D SCDPs systems. In every graph, demonstrate the comparison of thermal conductivity present results with previously known 2D SCDPs results that investigate through MD simulations techniques as GKR-EMD of Khrustalyov and Vaulina [27] at the higher scaling factor ($\xi = \infty$), and NEMD simulation data of Hou and Piel [26].

Figures 1 and **2** display the normalized thermal conductivity (λ_0) calculated at higher Debye screening strengths ($\kappa = 4.5, 5, 5.5, 6$) with setting $N = 400$ particles [22]. These **Figures 1** and **2** have plotted between Coulomb coupling (Γ) parameter and normalized thermal conductivity (λ_0) taken along the axis, x and y, respectively. It is noted that our simulation results are in better accordance with the earlier known numerical simulation results of 2D Yukawa liquids, at $N = 400$ [22]. It has investigated that, our new calculations for λ_0 at the lower value of

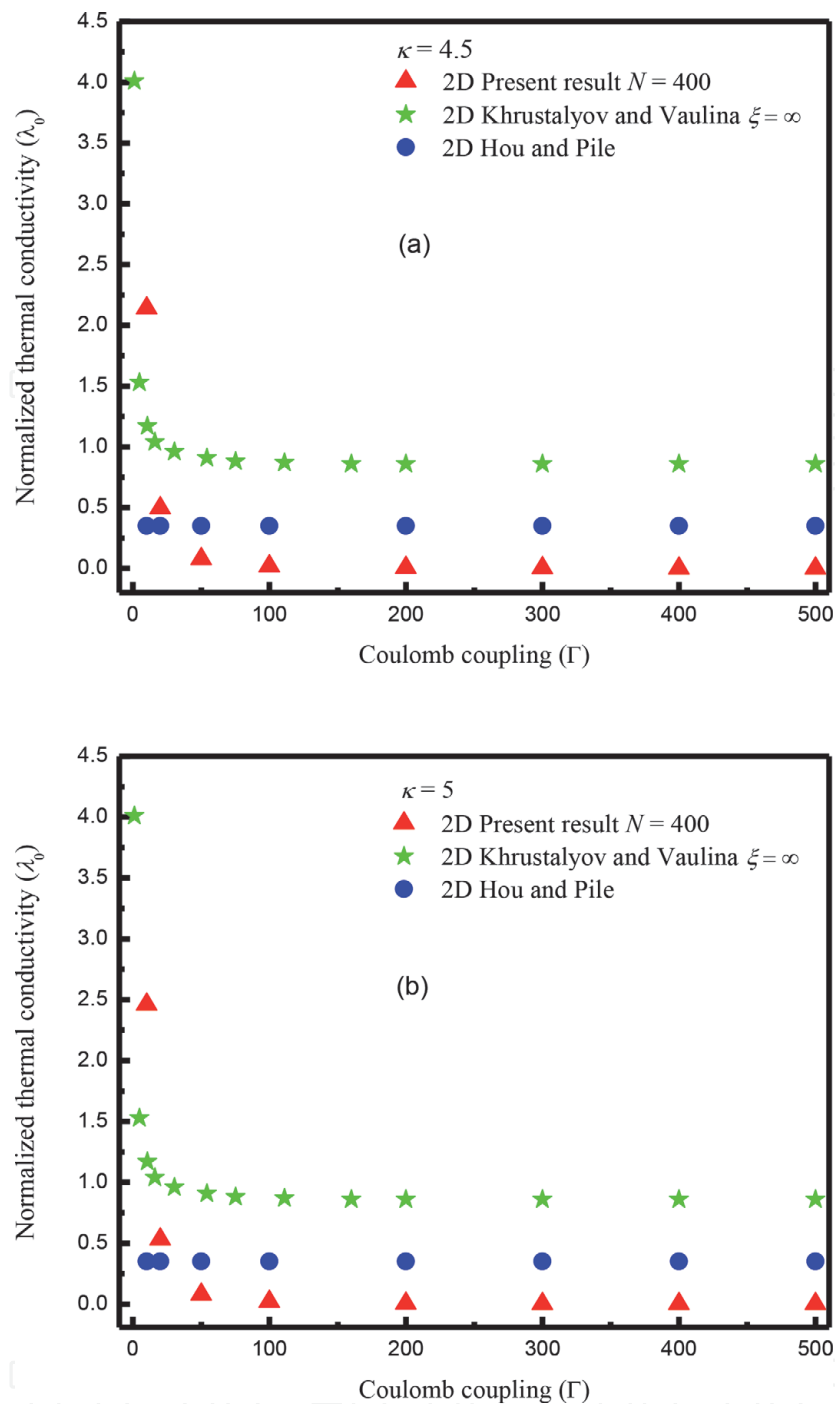


Figure 1. Normalized plasma thermal conductivity (λ_0) results from comparison versus coulomb coupling Γ ($10 \leq \Gamma \leq 500$) (system temperature) for SCCDPs computed from HNEMD at higher Debye screening, (a) $\kappa = 4.5$ and (b) $\kappa = 5$. Two-dimensional, GKR-EMD results of Khrustalyov and Vaulina (KV) [27] at the higher scaling parameter ($\xi = \infty$), and NEMD results of Hou and Piel (HP) [26]: current results (with 400 particles).

coupling Γ ($\equiv 20$) are lower than that of GK-EMD of Khrustalyov and Vaulina (KV) at the higher factor of scaling $\xi = \infty$ [27], and higher than 2D-NEMD estimations of Hou and Piel [26]. It is important to note that a constant behavior of λ_0 has examined at intermediate -higher Coulomb couplings ($50 \leq \Gamma \leq 500$) at constant force field $F^* \equiv 0.02$ [11], and well agreed with the previously known 2D SCDPs numerical simulation results of GKR-EMD [27] and NEMD [26] estimations. Moreover, it has observed that from the present simulation data, the existence of λ_0 is present for the entire range of plasma coupling Γ ($10 \leq \Gamma \leq 500$) at higher Debye screening (κ). The remains within an acceptable limited statistical uncertainty and also confirming the earlier computer simulation calculations of

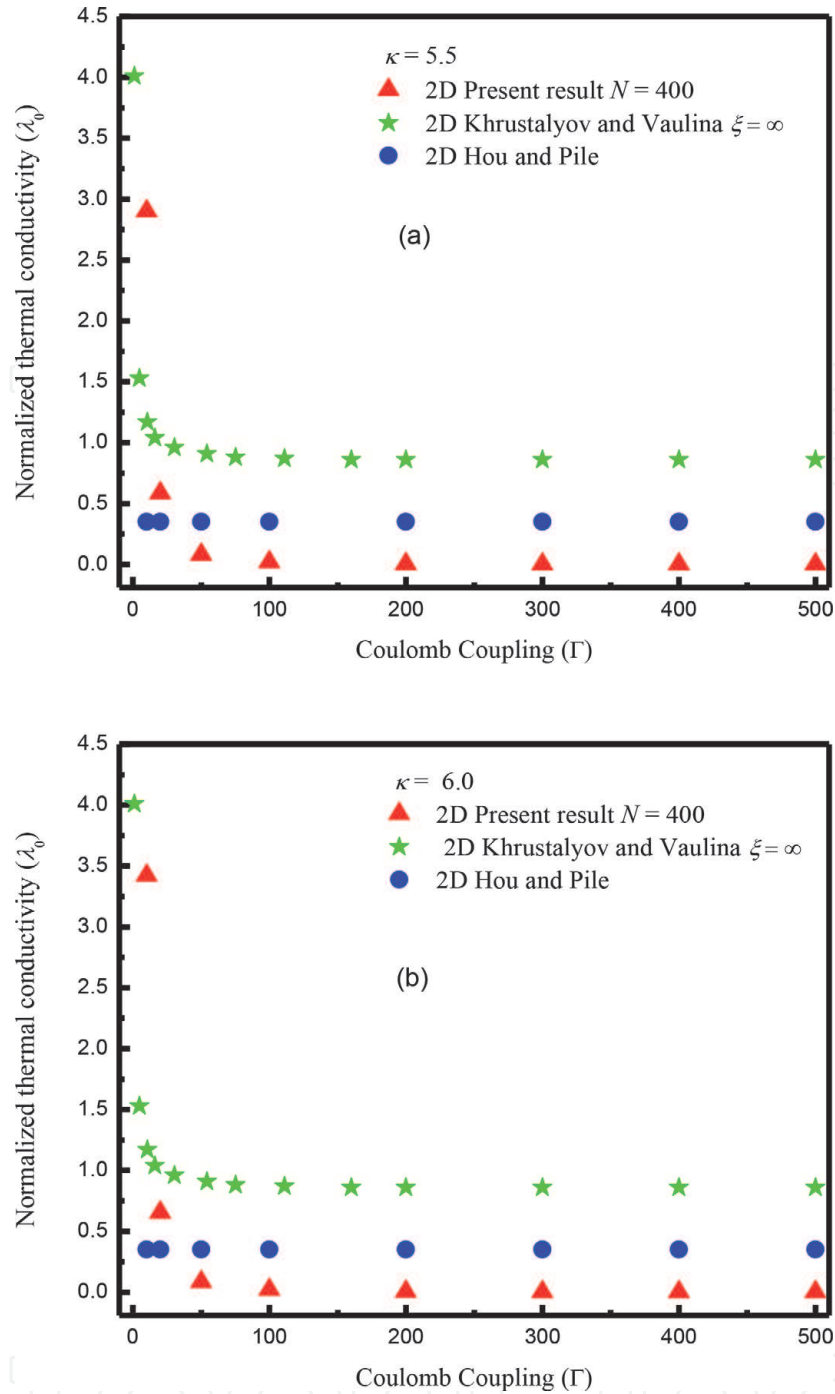


Figure 2. Normalized plasma thermal conductivity (λ_0) results from comparison versus Coulomb coupling Γ ($10 \leq \Gamma \leq 500$) (system temperature) for SCCDP_s computed from HNEMD at higher Debye screening, (a) $\kappa = 5.5$ and (b) $\kappa = 6$. Two-dimensional, GKR-EMD results of Khrustalyov and Vaulina (KV) [27] at the higher scaling parameter ($\xi = \infty$), and NEMD results of Hou and Piel (HP) [26]: current results (with 400 particles).

Shahzad and He [22]. The present simulation results show that the λ_0 decreases towards the higher Γ along with increasing the Debye screening (κ) [13]. It has investigated that our calculation of λ_0 for the lower value of Γ indicates that the interactions between the particles are very feeble, and the effectiveness of the screening parameter is large, and the K.E of particles is maximum. At intermediate-higher plasma coupling ($50 \leq \Gamma \leq 500$), the present results are below than the earlier 2D GKR-EMD numerical results of Khrustalyov and Vaulina [27] at the higher parameter of scaling $\xi = \infty$ [11], and 2D NEMD simulation estimations of Hou and Piel [24]. It has also observed that the presented simulation results are in better accordance with the previously known numerical results of 2D

Yukawa liquids at a normalized constant force field strength of $F^* = 0.02$. It is noted from these figures, our 2D HNEMD simulation results of λ_0 at the higher value of Debye screenings ($\kappa = 4.5, 5, 5.5, 6$) existing from nonideal state $\Gamma (=10)$ to a strongly coupled liquid state $\Gamma (=180)$ and further strongly coupled liquid state $\Gamma (=180)$ to strongly coupled solid-state ($180 \leq \Gamma \leq 500$). **Figures 1** and **2** show that the λ_0 exists for lower plasma coupling $\Gamma \leq 20$, which is the clear contradiction with the previously known simulation results of Donkó and Hartmann [13] where the λ_0 have not found at $\Gamma \leq 20$. Moreover, **Figures 1** and **2** show that the present simulation results have constant (straight line) behavior of λ_0 with increasing coulomb coupling (Γ). For higher Debye screening (κ) values for 2D SCDPs, that is the unlike to the simulation results of Shahzad and He [22], where the λ_0 displays a slightly growing behavior with increasing Γ for $\kappa = 4$. The possible reason for the difference between the present results and the previously known results of λ_0 may be the numerical error among HNEMD, NEMD, and GKR-EMD data.

It has proposed from these figures that measured results of λ_0 are in good accordance with earlier results at intermediate-high Γ . Nonetheless, a few outcomes veer at the lower Γ points; however, all within the statistical limited uncertainty range. **Figures 1** and **2** demonstrates that the presented HNEMD approach may accurately calculate the plasma thermal conductivity of strongly coupled complex (dusty) plasmas. We have shown that the present approach has excellent execution, and its exactness is exceptionally near to prior EMD and NEMD methods. It has concluded that our results rely upon the plasma parameters of Coulomb coupling and Debye screening strength, affirming previous simulations. Besides, it has demonstrated that the position of minimum value of thermal conductivity shifts towards higher Γ with an increase in κ , as expected in earlier numerical approaches. It is noticed that the improved HNEMD method is excellent for lower system sizes with constant external force field strength, where the signal to noise ratio is acceptable for equilibrium plasma thermal conductivity [31–33].

4. Summary

In this work, we have derived the plasma thermal conductivity of 2D SCDPs liquids over a suitable range of plasma couplings ($10 \leq \Gamma \leq 500$) and screening strengths ($4.5 \leq \kappa \leq 6$) at constant external force field strength by using HNEMD approach. Calculations have carried out employing HNEMD are in reasonable agreement with the earlier results measured from EMD and NEMD for SCDPLs. New investigations show that the minimum values of thermal conductivity shifts towards higher Γ with an increase of screening κ but remains within a reasonably limited statistical uncertainty, confirming the earlier simulation results. It has shown that the plasma thermal conductivity depends on plasma parameters (Γ, κ) in 2D complex dusty systems that illustrate earlier results of SCCDPLs. This chapter provides the understanding and investigation of the nonlinear regime of the SCCNPs for a suitable low value of external force field strength. In future work, the newly obtained results for thermal conductivity may be advantageous for developing new techniques of complex (dusty) plasmas diagnostics and also for improving the current experimental techniques for understanding the many nonideal systems like dusty plasmas, polymers, and biological and medical solutions. The remarkable outputs obtained from the successful development of employed model and can be used by the research labs and academia for their validation. The general experimentation on small scale and later on technological trials in industries will lead to the use of this plasma property for technology development purpose.

Acknowledgements

The authors thank Z. Donkó (Hungarian Academy of Sciences) for providing his thermal conductivity data of Yukawa Liquids for the comparisons of their simulation results, and useful discussions. They are grateful to the National Advanced Computing Center of National Center of Physics (NCP), Pakistan, for allocating computer time to test and run their MD code.

Abbreviations

SCCNPs	strongly coupled complex nonideal plasmas
HNEMD	homogeneous nonequilibrium molecular dynamics
Γ	Coulomb coupling
κ	Debye screening length
F^*	external force field strength
HNEMD	homogenous nonequilibrium molecular dynamics
NEMD	nonequilibrium molecular dynamics
MD	molecular dynamics
InHNEMD	inhomogenous nonequilibrium molecular dynamics
SCP	strongly coupled plasma
EMD	equilibrium molecular dynamics
λ	thermal conductivity
λ_0	normalized thermal conductivity
PBCs	periodic boundary conditions
VP	variance procedure
HPMD	homogenous perturbed MD
N	number of particles

IntechOpen

Author details

Aamir Shahzad^{1,2*}, Muhammad Qasim Khan¹, Muhammad Asif Shakoori²,
Maogang He² and Yan Feng³


¹ Molecular Modeling and Simulation Laboratory, Department of Physics,
Government College University Faisalabad (GCUF), Faisalabad, Pakistan

² Key Laboratory of Thermo-Fluid Science and Engineering, Ministry of Education
(MOE), Xi'an Jiaotong University, Xi'an, People's Republic of China

³ Center for Soft Condensed Matter Physics and Interdisciplinary Research, College
of Physics, Optoelectronics and Energy, Soochow University, Suzhou, China

*Address all correspondence to: aamirshahzad_8@hotmail.com;
aamir.awan@gcuf.edu.pk

IntechOpen

© 2020 The Author(s). Licensee IntechOpen. This chapter is distributed under the terms
of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/3.0>), which permits unrestricted use, distribution, and reproduction in any medium,
provided the original work is properly cited. 

References

- [1] Fortov VE, Vaulina OS, Lisin EA, Gavrikov AV, Petrov OF. Analysis of pair interparticle interaction in nonideal dissipative systems. *Journal of Experimental and Theoretical physics*. 2010;**110**:662-674
- [2] Wakeham WA, Nagashima A, Sengers JV. Measurement of the transport properties of Fluids. In: *Experimental Thermodynamics*. Vol. 3. Malden, MA: Blackwell Science; 1991
- [3] Qin G, Qin Z, Yue S-Y, Yan Q-B, Ming H. External electric field driving the ultra-low thermal conductivity of silicene. *Nanoscale*. 2017;**9**(21):7227-7234
- [4] Khan H, Haneef M, Shah Z, Islam S, Khan W, Muhammad S. The combined magneto hydrodynamic and electric field effect on an unsteady Maxwell nanofluid flow over a stretching surface under the influence of variable heat and thermal radiation. *Applied Sciences*. 2018;**8**(2):160
- [5] Chen FF. *Introduction to Plasma Physics and Controlled Fusion*. 2nd ed. New York: Springer Verlag; 2006
- [6] Chen FF. *Industrial Applications of Low-Temperature Plasma Physics*. Los Angeles: University of California; 1995. pp. 90024-91594
- [7] Killian T, Pattard T, Pohl T, Rost J. Ultracold neutral plasmas. *Physics Reports*. 2007;**449**:77
- [8] Piel A. *Plasma Physics: An Introduction to Laboratory, Space, and Fusion Plasmas*. Heidelberg, Berlin: Springer Science & Business Media; 2010. pp. 1-378. DOI 10.1007/978-3-642-10491-6
- [9] Merlino RL. Dusty plasmas and applications in space and industry. *Plasma Physics Applied*. 2006;**81**:73-110
- [10] Frenkel D. Simulations: The dark side. *The European Physical Journal Plus*. 2013;**128**(1):10
- [11] Shahzad A, Haider SI, Kashif M, Shifa MS, Mu T, He MG. Thermal conductivity of complex plasmas using novel Evan-Gillan approach. *Communications in Theoretical Physics*. 2018;**69**(6):704
- [12] Shahzad A, Shakoori MA, He MG, Yang F. Dynamical structure factor of complex plasmas for varying wave vectors. *Physics of Plasmas*. 2019;**26**: 023704
- [13] Donkó Z, Hartmann P. The thermal conductivity of strongly coupled Yukawa liquids. *Physical Review E*. 2004;**69**(1):016405
- [14] Ott T, Bonitz M. Effective coupling parameter for 2D Yukawa liquids and non-invasive measurement of plasma parameters. 2010. arXiv preprint arXiv: 1010.6193
- [15] Shahzad A, He MG, Irfan Haider S, Feng Y. Studies of force field effects on thermal conductivity of complex plasmas. *Physics of Plasmas*. 2017;**24**(9):093701
- [16] Shahzad A, He MG. Thermal conductivity of three-dimensional Yukawa liquids (dusty plasmas). *Contributions to Plasma Physics*. 2012; **52**(8):667-675
- [17] Shahzad A, He MG. The numerical experiment of thermal conductivity in two-dimensional Yukawa liquids. *Physics of Plasmas*. 2015;**22**(12):123707
- [18] Hansen JP, McDonald IR. *Theory of Simple Liquids*. London: Academic; 1986 (1976; Google Scholar: 179)
- [19] Shahzad A, He MG. Thermal conductivity calculation of complex (dusty) plasmas. *Physics of Plasmas*. 2012;**19**(8):083707
- [20] Shahzad A, Aslam A, He MG. Equilibrium molecular dynamics simulation of shear viscosity of

two-dimensional complex (dusty) plasmas. *Radiation Effects and Defects in Solids*. 2014;**169**(11):931-941

[21] Shahzad A, He MG. Interaction contributions in thermal conductivity of three dimensional complex liquids. *AIP Conference Proceedings*. 2013;**1547**: 172-180

[22] Shahzad A, He MG. Homogeneous nonequilibrium molecular dynamics evaluation of thermal conductivity in 2D Yukawa liquids. *International Journal of Thermophysics*. 2015;**36** (10–11):2565-2576

[23] Salin G, Caillol JM. Equilibrium molecular dynamics simulations of the transport coefficients of the Yukawa one component plasma. *Physics of Plasmas*. 2003;**10**(5):1220-1230

[24] Faussurier G, Murillo MS. Gibbs-Bogolyubov inequality and transport properties for strongly coupled Yukawa fluids. *Physical Review E*. 2003;**67**(4): 046404

[25] Donko Z, Hartmann P. Shear viscosity of strongly coupled Yukawa liquids. *Physical Review E*. 2009;**78**: 026408

[26] Hou LJ, Piel A. Heat conduction in 2D strongly coupled dusty plasmas. *Journal of Physics A: Mathematical and Theoretical*. 2009;**42**(21):214025

[27] Khrustalyov YV, Vaulina OS. Numerical simulations of thermal conductivity in dissipative two-dimensional Yukawa systems. *Physical Review E*. 2012;**85**(4):046405

[28] Evans DJ. Homogeneous NEMD algorithm for thermal conductivity—Application of non-canonical linear response theory. *Physics Letters A*. 1982;**91**(9):457-460

[29] Evans D, Morriss G. *Statistical Mechanics of Nonequilibrium Liquids*. London: Academic; 1990

[30] Shahzad A, Sultana M, Aslam A, He MG. Molecular dynamics simulations of thermal conductivity in 2D complex Yukawa liquids. *IOP Conference Series: Materials Science and Engineering*. 2013;**60**:012038

[31] Shahzad A. *Impact of Thermal Conductivity on Energy Technologies*. London: IntechOpen; 2018. DOI: 10.5772/intechopen.72471

[32] Shahzad A, Haider SI, He MG, Yang F. Introductory Chapter: A Novel Approach to Compute Thermal Conductivity of Complex System, a Chapter from the Book of *Impact of Thermal Conductivity on Energy Technologies*. London: IntechOpen; 2018. 3 p. DOI: 10.5772/intechopen.75367

[33] Shahzad A, He M-G. Thermal Conductivity and Non-Newtonian Behavior of Complex Plasma Liquids, a Chapter from the Book of *Thermoelectrics for Power Generation—A Look at Trends in the Technology*. InTech: Rijeka, Croatia; 2016. p. 305. DOI: 10.5772/65563