Chapter

Studies of Self Diffusion Coefficient in Electrorheological Complex Plasmas through Molecular Dynamics Simulations

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Abstract

A molecular dynamics (MD) simulation method has been proposed for three-dimensional (3D) electrorheological complex (dusty) plasmas (ER-CDPs). The velocity autocorrelation function (VACF) and self-diffusion coefficient (D) have been investigated through Green-Kubo expressions by using equilibrium MD simulations. The effect of uniaxial electric field (M_T) on the VACF and D of dust particles has been computed along with different combinations of plasma Coulomb coupling (Γ) and Debye screening (κ) parameters. The new simulation results reflect diffusion motion for lower-intermediate to higher plasma coupling (Γ) for the sufficient strength of $0.0 < M \geq 1.5$. The simulation outcomes show that the M_T significantly affects VACF and D. It is observed that the strength of M_T increases with increasing the Γ and up to $\kappa = 2$. Furthermore, it is found that the increasing trend in D for the external applied M_T significantly depends on the combination of plasma parameters (Γ, κ). For the lower values of Γ, the proposed method works only for the low strength of M_T; at higher Γ, the simulation scheme works for lower to intermediate M_T, and D increased almost 160%. The present results are in fair agreement with parts of other MD data in the literature, with our values generally overpredicting the diffusion motion in ER-CDPs. The investigations show that the present algorithm more effective for the liquids-like and solid-like state of ER-CDPs. Thus, current equilibrium MD techniques can be employed to compute the thermophysical properties and also helps to understand the microscopic mechanism in ER-CDPs.

Keywords: Diffusion coefficient, electrorheological complex plasma, Molecular dynamics simulations, uniaxial electric field

1. Introduction

1.1 Electrorheological fluids

The dielectric fluids consisting of micro-sized (0.1-100 μm) solid particles, which display particular characteristics under the influence of the external applied electric field, are known as electrorheological fluids (ERFs). The dielectric fluids, such as olive oil, silicon oil hydrocarbon, etc., have low permittivity, conductivity and viscosity. The solid particles immersed in dielectric fluids are mostly polymers, metal oxide silica, and alumina silicates. These particles maintained the low viscosity of carrier fluids in the absence of external electric field strength. Without an external electric field, particles behave as a liquid. When the external electric field is turned on, these particles behave like solids due to changes in viscosity. The ERFs change their physical properties for the application of the external electric field. When the electric field is turned on the suspension of dielectric fluids, the solid particles are polarized and make a thin chain (string) along the direction of the applied electric field. The thickness of the particles depends on the intensity of the electric field. The viscosity of ERFs increased with increases an external applied electric field. If the electric field was turned off, the fluids reverse from solid to liquids within milliseconds. These fluids are also known as intelligent fluids. There are various types of rheological fluids, such as electrorheological fluids, magnetorheological fluids, positive electrorheological, negative electrorheological fluids etc. These fluids rapidly respond to the electric field and change their physical properties such as shear stress, elastic modulus and viscosity. These fluids are used in vehicle engineering, such as valves, clutches and breaks etc. The conventional ERFs have various industrial applications, such as vibration control in smart materials. Changes in the microstructure and physical properties are used in medical to control ultrasonic transmissions and sound transmission with low losses [1, 2].

1.2 Plasma

Plasma is a partially ionized gas that contains electrons, ions and neutral radicals. In our universe, 99% of physical matter is in the plasma state. In space, the most visible matter is in the plasma state; the sun and stars are the main examples of plasma in our universe. Plasma species show collective behaviors when any external perturbation is applied. The whole plasma is perturbed when an external force has applied this behavior of particles called collective behavior of plasma. Classification of plasma depends on the species temperatures such as hot plasma, cold plasma, ultracold plasma, ideal and non-ideal plasma etc. [3].

1.2.1 Complex (dusty) plasmas

Complex (dusty) plasmas (CDPs) contained micro to submicron-sized conductive, and dielectric particles called grain in addition to plasma species (neutral atom, electron, positive or negative ions). The conductive grain has a $3e^{-11}$ kg mass and about e^4 eV charge. Mostly having a negative charge but in the rear case also have positive charge depend on charging phenomena. Dust particles are naturally present in the plasma and can be manually inserted in a plasma medium through sputtering, etching and chemical reaction—the dust particles made by a single element or composition of different elements. The dust particles like a swimmer in the sea of electrons and ions and respond to electromagnetic forces. There are different mechanisms of charging dust particles. The charge amount depends on the charging phenomena. Dusty plasmas illustrate an astrophysical matter in white dwarfs, neutron stars, giant planetary interiors and supernova core. In laboratory ultra-cold plasma, charged stabilized collides and electrolytes, laser-cooled ions in cryogenic traps, and dusty plasma. The warm dense matter and strongly coupled complex (dusty) plasmas (SCCDPs) are relevant models for nuclear fusion devices [3–6].

The CDPs are classified according to the energies of interacting charged dust particles. When interacting particle's potential energy exceeds their kinetic energy, then CDPs are called as SCCDPs. This system appears in a wide variety of physical systems. The Weakly coupled complex (dusty) plasmas (WCCDPs) are inverts of SCCDPs. The SCCDPs also in high order structural form or exist in the crystalline state at low temperature with high density. The WCCDPs are mostly remained in the gaseous state of the plasma and having high temperature with low density. Various states of dusty plasma are easily observed through a video camera under laboratory conditions. SCCDPs are found in nature and also in laboratory experiments [7, 8]. The phase transition (condensation) can be observed by reducing the temperatures of CDPs. The structural order of dust particles is formed under some external conditions. The dusty plasmas are encountered in astrophysics and are extensively believed to play a significant role in cosmology to reveal the structure and origin of the universe and its galaxies. The transport and thermodynamic properties are well studied for CDPs through experiment, theoretical and computational methods. Thermophysical properties are well investigated in the recent decade, such as thermal conductivity [9–11], diffusion phenomena [12, 13], shear viscosity [13], thermodynamic properties [14], dynamical structure factor [4, 15] and propagation of different waves [3, 5].

1.3 Applications of complex dusty plasmas

Initially, CDPs originate in astrophysics and space physics; nowadays, it becomes a fascinating, applicable field in space physics as an analogue to unravel issues like the role of dust accumulation super high speed crashed in space and the formation of planets and many industries on different scales. The CDPs play an essential role as an analogue system for investigating multifaceted cross-disciplinary phenomena, such as an experimental study of non-linear dynamics and long-range interaction in strongly correlated systems. These systems often have challenging investigations because they generally require extreme temperature and pressure conditions, such as very low temperature and high density. These systems belong to different research institutes. The CDPs allow the study and formation of the strongly coupled systems under laboratory conditions at room temperature and for easily attainable pressure. The CDPs analogue was recently used to model crystallization dynamics in 2D and excitation of quantum dots, viscoelastic material, shock and non-linear waves and recently electrorheological fluids [16].

In industrial applications, CDPs are directly applicable in the processing of microelectronics devices. It is used for deposition integrated circuits, masking, and stripping. The capacitors and transistors make on the silicon wafer chip millions of transistors put on the Pentium chip with the help of plasma to safe from contaminations. Dust particles have both advantages and disadvantages in the technologies. It plays a vital role in the scientific research of various technologies and industries. It plays a significant role during the thin-film depositions, processing of ceramic, insulation, filtration processes, petroleum industry, biomechanics, paper industry, packed bed reactors etc. Dust particles are helped to enhance the efficiency and stability of solar cells, LED (light emitted diode), improving lighting source, display, and laser technology. Through plasma processing, the coating of particles has been produced. It has grown or modified existing materials in the semiconductor industry [17]. The scientific communities currently focus on controlling nuclear fusion reactions and developing devices such as tokamak to produce efficient and carbon-free energy.

In the field of medicine and healthcare, the CDPs have become an emerging field, which combines plasma physics, life science, and clinical medicine. In the area of life science, it is directly used in biological medicine such as double-helix molecular interaction, sterilizing surgical instruments and implants, wound healing, cancer therapy, break DNA damage for human prostate cancer [18]. The CDPs were found to help kill cancer cells without affecting the healthy tissues. It is also used to inactive the bacterial in the field of health care. It is also used for food storage technologies. Furthermore, the CDPs are helpful as a diagnostic technique for a precise calculation of plasma parameters such as non-linear laser spectroscopy, spectrally resolved nanosecond imaging, phase-resolved optical emission spectroscopy, and laser-induced fluorescence VUV, UV, VIS and IR, etc. [19].

1.4 Electrorheological complex dusty plasma

CDPs have electrorheological characteristics like conventional electrorheological fluids when an external ac electric field is applied. The dust particles respond quickly to the external applied electric field and make a chain (string) sheet-like as conventional ERFs so-called electrorheological CDPs (ER-CDPs). The first time ER-CDPs were observed by Ivlev A. V. et al., in 2008 during the microgravity experiments (PK-3 plus laboratory) and MD simulation. They show the phase transition of CDPs from isotropic to anisotropic with increasing the external applied electric field [20]. Under the influence of electric field dc mode, attractive attractions between charged dust particles are introduced by ions streaming. In this way, wake potential behind the dust grains produced, which make particles strings (sheet), in the dc discharge plasma sheath, where charged dust particles levitated against the electric field's gravity force. Such a type of system is non-Hamiltonian, and wake potential is asymmetric. The ac electric fields have a much smaller frequency than ion plasma frequency, but larger than dust plasma frequency was applied to the complex plasma. In this way, the wake potential is symmetric, and a system known as Hamiltonian due to the electric field, dipole–dipole attractions increased in ER-CDPs, particles arrange themselves in sheet, string, or crystalline structure same as conventional ERFs. The phase transition in ER-CDPs has studied experiments and simulations method [20–23].

After discovering ER-CDPs, it opens up new dimensions of research for plasma science and technologies communities. There is little literature available to understand the macroscopic phenomena of ER-CDPs. Ivlev A. V. et al., done a PK-3 plus experiments under microgravity conditions and molecular dynamics simulations, observed phase transition from an isotropic to string with increasing external ac electric field [24]. Later they have done *PK*-4 dc discharge experiment and observed an anisotropic structure under the influence of an external ac electric field [22]. Yaroshenko V. V. theoretically studied the propagations of dust lattice waves along the electric field in a one-dimensional string. He found the instability leads to spontaneous excitations of compressional waves [25]. Rosenberg *M*. theoretically studied the formation and excitation of waves in one-dimensional ER-CDPs under the ac electric field [26]. Kana *et al*. explored the phase transition in ER-CDPs using MD simulation and observed the anisotropic structure under the influence of ac electric field and did not find the anisotropic structure for the dc electric field mode [21]. Sukhinin *et al*. used a Monte Carlo (MC) simulation of plasma polarization around dust particles in an external applied electric field. They mentioned that due to induced dipole potential, the formation of dust particles alignment, chain (string) multi-layered structure, and coagulation of charged dust particles [27]. A self-consistent model was developed for plasma anisotropy (string) of charged dust particles under the external electric field's action by Sukhinin *et al*. [28]. No evidence has been found of thermophysical properties in ER-CDPs. In the future, for precise tailoring, new materials may be modeled with the help of ER-CDPs. The ER-CDPs can play a significant role in modeled new smart materials. It is also be used to generate negative dipolar interparticle interactions [24].

1.5 Diffusion coefficient

The diffusion coefficient is one of the transport properties of gas, liquids. During the diffusion process, the particles migrate from high concentrations to low concentrations. The diffusion rate can be controlled by variations of external parameters such as temperature, concentration, external electromagnetic forces (electric and magnetic). Investigations of diffusion have different purposes in liquids, such as exploring the dynamical properties and understanding the microscopic phenomena. For the CDPs research direction, the investigations of diffusion motion for applying external fields such as electric and magnetic become a hot topic in current research. Different types of diffusion motion exist in dusty plasma regimes depends on temperature and forces. Diffusion also plays an essential role in exploring the dynamical properties (structure, waves, and instabilities) of many biological, physical, and chemical systems. The diffusion motion of dust particles in CDPs continues as one of the active research topics, an essential consequence of understanding the transport and dynamical properties [12, 29–33]. It is one of the primary sources to lose energy (stopping power) in CDPs. Therefore, we can easily understand the microscopic phenomena of particles in the different states [34]. An extensive amount of previous studies have been made to understand the diffusion motion in CDPs. Molecular dynamics simulations were performed and investigate the velocity autocorrelation function for 2D WCCDPs [12], Langevin dynamics simulation for 2D SCCDPs [35] and diffusion coefficient [36]. For the investigations of self-diffusion coefficient MD simulations were performed for 3D CDPs [30, 33, 37], one-component plasma [31] and ionic mixtures [32].

The main objective of the present book chapter is to give an overview of electrorheological (ER) fluids and ER-CDPs. We have computed the effect of the external applied uniaxial electric field on the velocity autocorrelation function and self-diffusion coefficient of 3D ER-CDPs using MD simulations over a wide range of input CDPs parameters.

2. MD simulation algorithm and parameters

The Computer simulation provides a linkage between theoretical and experimental research work. In thermal fluids, science and engineering, the installations of experimental setups are very complex and high cost. In the age of modern technology, the cost-effective and low time consumption high computational power is most prominent. Nowadays, it is a trend that before starting the experimentations, first test with computational tools than verified with experiments. There are various computer algorithms and techniques are used for the calculation of various properties in various materials. We perform computer simulations to test a theoretical model, verify experimental data, and also for comparison purposes [38]. Different computational techniques can be designed for extreme conditions, such as for very low temperature and high density. It also acts as a bridge between microscopic length, time scale, and macroscopic worlds. MD and Monte Carlo (MC), and Langevin dynamics simulations are the main methods used to compute CDPs' physical properties. Different software's are also available to compute various physical properties and build a new model by following one simulation scheme.

MD simulations have become a prominent computational tool to investigate various properties such as thermophysical and dynamical properties in different types of fluids and materials. The MD simulations consist of the numerical solution of the Newton equation of motion for the spherical particles system [9]. This section explained the MD simulation algorithm to calculate the self-diffusion coefficient (D). Equilibrium MD simulations are used to investigate the D in ER-CDPs. Yukawa potential (screened Coulomb) is the most commonly used potential for CDPs systems, while other physical systems such as physics of chemical and polymer, medicine and biology systems, astrophysics, and environmental research are adopted. Most scholars used Yukawa potential to screen charged dust particles in the dusty plasma results in isotropic interactions. In the present research used applied a uniaxial ac electric field for additional dipole–dipole-like interactions. This idea was taken from Pk-3 plus experiment under the microgravity conditions [20], theoretical approach [39], MD simulation study [24], and *Pk*-4 experiments [23]. For ER-CDPs, the charged dust particles interact with each other through Yukawa potential and Quadrupole interactions due to external applied ac electric field: the equation for ER-CDPs becomes as

$$W(r,\theta) = Q_d^2\left[\frac{1}{4\pi\varepsilon_o}\,\frac{\exp^{-r/\lambda_D}}{r} - 0.43\frac{M_T^2\lambda_D^2}{r^3}\left(3\cos^2\theta - 1\right)\right] \tag{1}$$

First-term in the above equation presents pair-wise Yukawa potential in the absence of an electric field, and the second term shows the Quadrupole interaction between particles due to uniaxial ac external electric field [22]. Where λ_D is Debye length, Q_d is the charge on dust particles, r distance between interacting particles, and ϵ_o permittivity of space. The θ is the angle between the electric field ($\boldsymbol{E}$) and interacting dust particles. In the present study, we take $\theta = 0^\circ$ for uniaxial ac electric field for anisotropic interactions. The $\boldsymbol{r}$ is the distance between the interacting particles, $\boldsymbol{r} = \boldsymbol{r}_j - \boldsymbol{r}_i$. The M_T is thermal Mach number normalized with the thermal velocity of charged dust particles $M_T^2 = \langle u_d^2\rangle / v_T^2$ where $v_T^2 = T_d/m_d$ the drift velocity is proportional to an electric field ($u_d \propto E$), an electric field can be measured in the unit of M_T. For small values of $M_{T,}$ in ER-CDPs, the interactions of particles are the same as dipolar interaction in conventional ERFs. In the prior study, strings (chain) of dust particles were observed in typical conditions when an external ac electric field was applied.

There are two central (dimensionless) parameters, which are fully-characterized complex plasma systems. The first parameter is the plasma coupling parameter (define same as Coulomb systems) $\Gamma = Q_d^2/4\pi\epsilon_o a_{w.s} k_B T$, a_{ws} Wigner-Seitz radius defined as $(3/4\pi n)^{\frac{1}{3}}\pi n^{\frac{-1}{2}}$ Where n is the equilibrium dust number density, k_B the Boltzmann constant, and T is the system's absolute temperature. The plasma coupling (Γ) parameter is the ratio of average potential energy to the average kinetic energy of interacting dust particles. The SCCDPs associated with $\Gamma > 1$ inversely account as weakly coupled dusty plasma ($\Gamma < 1$). Another essential parameter is the Debye screening parameter, $\kappa = a_{w.s}/\lambda_D$. The plasma dust frequency $\omega_{pd} = \left(Q_d^2/3\pi\epsilon_0 m a^3\right)^2$ describes the time scale of a complex plasma system; here, m is the dust particle's mass.

2.1 Green-Kubo relation of diffusion coefficient

Green-Kubo integral formula were used to calculate the self-diffusion coefficient (D) for 3D CDPs [30, 33], one component plasma [31] and ionic mixtures [32]. Here we have used the same numerical models for the investigations of D in 3D ER-CDPs; the Green-Kubo relation is given as following.

$$D = \frac{1}{3N}\int_0^\infty Z(t)dt \tag{2}$$

In Eq. (2), $Z(t)$ is known as the velocity autocorrelation function (VACF), 3 shows the 3D system, and N represents the number of simulated dust particles. The D is the integral of VACF calculated over all the particle velocity product's ensemble average segments at a time (t) and initial time (t_0). If $Z(t)$ decays too slowly, Yukawa particles' motion is described as anomalous diffusion for the integral equation one converges. The transport coefficient's existence, autocorrelation function must rapidly decay enough for integral to convergence. Different types of diffusion motion were analyzed through VACF [12], defined as

$$Z(t) = \langle v_j(t).v_j(0) \rangle \tag{3}$$

Where $v_j(t)$ denote the j^{th} particle's velocity at simulation time (t) and (0), the brackets $\langle . \dots \rangle$ represent the canonical ensemble average all over particles. $Z(t)$ demonstrates the decay that is characterized by plasma frequency. The existence of the transport coefficient, autocorrelation function must rapidly decay enough for integral convergence [29, 33, 34].

In this method, classical molecular dynamics simulations are used to map the trajectories of N = 500 and calculated the diffusion coefficient. Periodic boundary conditions (PBCs) were used to be constrained enforced during the N-particles simulation under statistical microcanonical ensemble (NVE). The edge length of the 3D cubic simulation box is L with 12.79a. Particles are placed randomly in the simulation cubic cell for the beginning of the simulations [15]. An appropriate time step (dt = $0.001\omega_{pd}$) was selected to calculate particle position and velocity at each step. The leapfrog integration method is used to integrate the equation of motion and calculate each particle's force, acceleration, and position for every time step. The whole scheme in MD dynamically simulates the equation of motion of N-dust particles with interaction through Yukawa potential, and Quadrupole interaction was given in Eq. (1). The Ewald summation method was used for calculations of Yukawa and dipolar potential energies and forces. Here we select the Ewald convergence parameter (γ = 5.6/L) for the Yukawa and anisotropic interactions. Suitable input parameters are selected to get the accuracy and consistency of the model. The appropriate system temperature (($T = 1/\Gamma$) Yukawa Ewald-summation method, screening length, Mach number, time step, number of particles, simulation run time, etc., are selected to provide 3D ER-CDPs diffusion motion. Negative derivatives of Eq. (1) calculate forces on each interacting charged dusty particle in the Yukawa system. MD simulations are performed 2 x $10^5/\omega_{pd}$ time unit to record the SDC (Γ, κ, M_T). The 12-core-processor takes about three hours to perform each simulation. Total 156 simulations are performed and calculated the VACF and D for a wide range of plasma parameters and external applied uniaxial electric field. For the present chapter, the EMD method is used of ER-CDPs and calculated the D over a wide range of Γ = 2–500, $1 < \kappa \geq 3$, and N = 500. In addition, the conservation of total energies and momentum is checked and verify that system has self-consistency.

3. Simulation results and discussions

This book chapter used the equilibrium MD simulation method using Yukawa (screened Coulomb) potential and dipolar interactions. Without external forces (electric and magnetic), Yukawa potential was used and calculated thermophysical properties. In this work, we add dipolar interactions with the same numerical schemes and analyses the diffusion motion through VACF and D. First of all; we compute the VACF for Screening parameters ($1 < \kappa \geq 3$), plasma coupling parameters ($1 < \Gamma \geq 500$), uniaxial electric field strength ($0.0 \leq M_T \geq 1.50$) for the same number of particles (N = 500). After that, D is calculated for nearly the same parameters used for the VACF.

The single-particle motions are computed for 3D ER-CDPs through the equilibrium MD simulation using VACF for diffusion by employing Eq. (3). VACF are analyzed and discussed for plasma screening κ = 1.4, 2 and 3, plasma coupling (Γ = 2–500), number of spherical charged dust particles (N = 500) with the variation of the external uniaxial electric field. The VACF has been widely used for 3D CDPs over a wide combination range of plasma parameters (κ, Γ) [12, 30, 36]. The VACF was computed at M_T = 0.0 for comparison purposes with earlier MD results. It has been shown that MD outcomes have comparable fair agreements with previous results. Here we defined the critical strength of the applied external electric field (M_{CT}). The M_{CT} is directly proportional to plasma coupling strengths or inversely proportional to system temperature. We have been found that above the M_{CT} system goes out of thermal equilibration. We have also got noisy results above the M_{CT} strength of the external applied uniaxial electric field. The critical strength of the uniaxial electric field is different for the different combinations of CDPs parameters.

The simulation outcomes of VACF in 3D ER-CDPs as a function of the simulation time scale for four different plasma coupling values ($\Gamma \equiv$ 20, 50, 100, and 250) at constant κ = 1.40 and N = 500 are displayed in **Figure 1**. The effects of variation uniaxial electric field ($M_T \equiv$ 0.01–1.30) on VACF are computed to analyze the diffusion motion of charged dust particles. It has been shown that M_T significantly depends on plasma temperature and the screening of charged particles. At Higher plasma temperature (Γ = 20), one can easily observe the rapid decay of VACF with very weak particle oscillations. This regime M_T does not have significant effects on the dynamics of dust particles. **Figure 1(b)** shows the oscillatory damped motion and slightly decreasing amplitude of VACF up to uniaxial electric field strength (M_T = 0.90). For higher plasma coupling strength ($\Gamma \equiv$ 100,250), results of VACF show the higher oscillations with slightly damping phenomena. **Figure 2** demonstrated the VACF at κ = 2.0 for four different regimes of strongly coupled CDPs (Γ = 20, 50, 200, 400) N = 500 with a variation of uniaxial electric field ($0.0 < M_T \geq 1.50$). It is observed that the effect of M_T on VACF is nearly the same as was observed in **Figure 1**. It has also been shown that the M_{CT} increases with increases in the screening strength. Furthermore, we increased the screening strength κ = 3.0 and Γ = 30, 75, 250, and 500 are shown in **Figure 6**. The trend of damping and oscillations of dust particles was observed the same as in **Figures 1** and **2**. Therefore, the VACF below the M_{CT} simulation outcomes is founded in good agreement with previous data [13, 30, 35, 36].

It is observed that at higher temperatures (low coupling, Γ), the M_T does not affect the dynamics and oscillation of the particles. So what we can say that at higher system temperature, the radius between interacting charged dust particles is large. Due to the large distance, Eq. (1) remains invalid for higher uniaxial electric field strength. The motion of a particle in this regime indicates only thermal motion. Complete damped oscillations of dust particles were observed for a long time at intermediate values of Γ. The magnitude of oscillations slightly decreased with increasing M_T, increasing the diffusion at a low rate of thermal motion. In ER-CDPs, the effect of M_T on VACF can be easily observed from intermediate to higher plasma coupling (Γ) strength. The simulation time length scales, maximum at intermediate values of Γ and further increasing Γ, the length scale slightly decreased. It was observed that the oscillation was not fully damped at higher Γ. It is concluded that a uniaxial electric field can affect diffusion motion in ER-CDPs for the sufficient strength of M_T., so what can say the presented numerical method gives us precise and reliable data for comparative study.

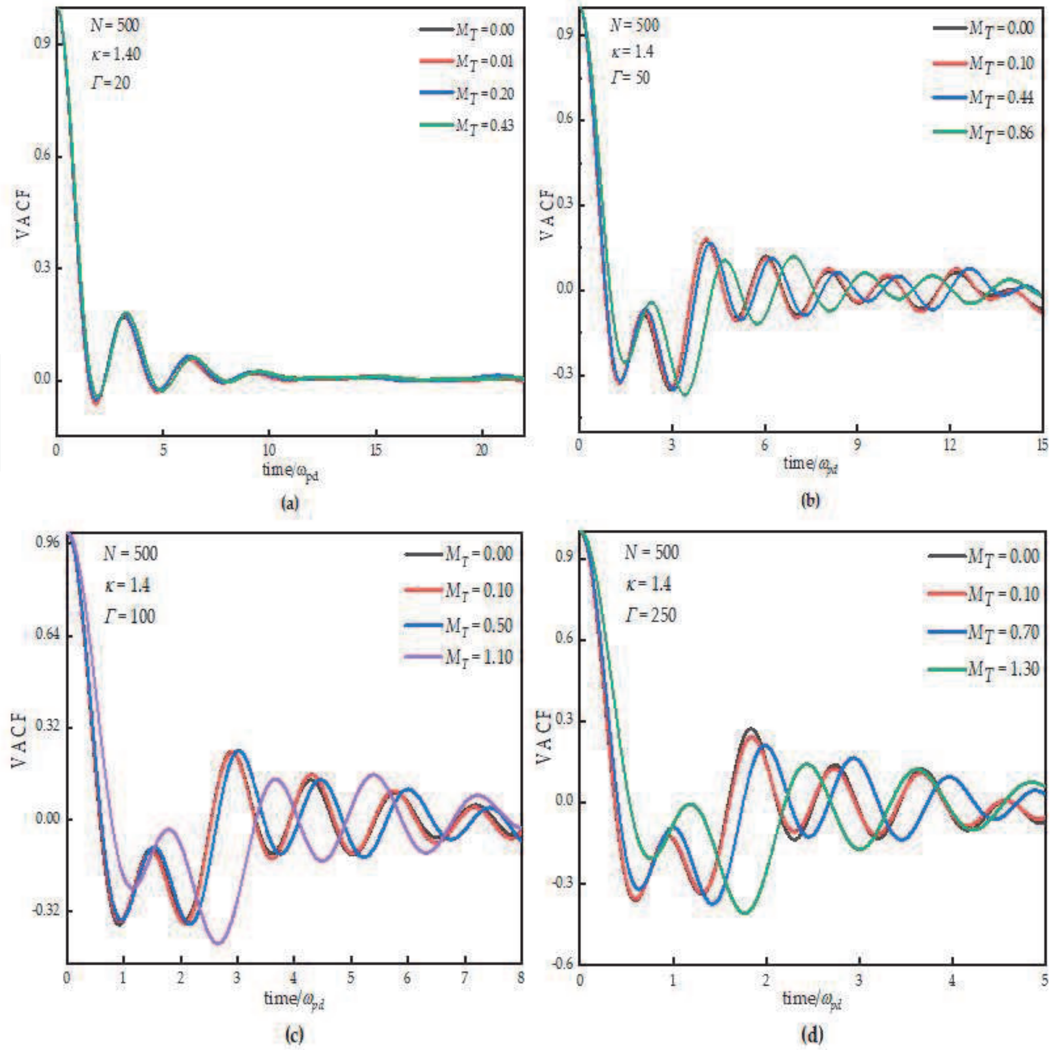

Figure 1.
VACF as a function of molecular dynamics simulation time scale for constant plasma screening parameter (κ = 1.40). MD simulations results obtained for N = 500 *simulated dust particles with the variation of uniaxial external electric field (0.0 <* $M_T \leq$ *1.30) and four different plasma regimes (a)* Γ = 20, *(b)* Γ = 50, *(c)* Γ = 100 *and (d)* Γ = 250.

Now we focused on the primary outcomes through the equilibrium MD method. The simulation data of this work are that the self-diffusion coefficient (D) of ER-CDPs can be obtained with minimum statistical error at M_T = 0.0 by equilibrium MD. Moreover, it is shown that the MD with GKR has a fair good agreement with previous simulation outcomes of Ohta and Hamaguchi [30], Daligault [31, 32], and Begum and Das [33, 37] at M_T = 0.0. **Figures 3–5** display the primary outcomes of D measured from the equilibrium MD method for ER-CDPs at κ = 1.4, 2, and 3, respectively. D of ER-CDPs was calculated for different uniaxial electric field strengths ($0 < M_T < 1.5$). Here we have explained the D for a wide range of combinations of plasma parameters (Γ, κ) over acceptable M_T ranges below the M_{CT}. This section focused on the variation of plasma coupling ($1/T$), electric field, Debye screening length, and constant N = 500 simulated particles.

The effect of M_T on D in 3D ER-CDPs is calculated for plasma coupling ($\Gamma \equiv 20$, 50, 100, and 200), Debye screening length ($\kappa \equiv 1.4$), uniaxial electric field ($0.0 \leq M_T \leq 1.30$), and N = 500 number of particles shown in **Figure 3**. We have performed several MD simulations at constant κ = 1.4 and N = 500 to analyze the effect of M_T on D. The reported data of D shows good agreements for small M_T values with previous results [30–32]. With respective of Γ different regimes are under consideration. It is found that the M_{CT} values are the same as in **Figures 1, 2, 6**

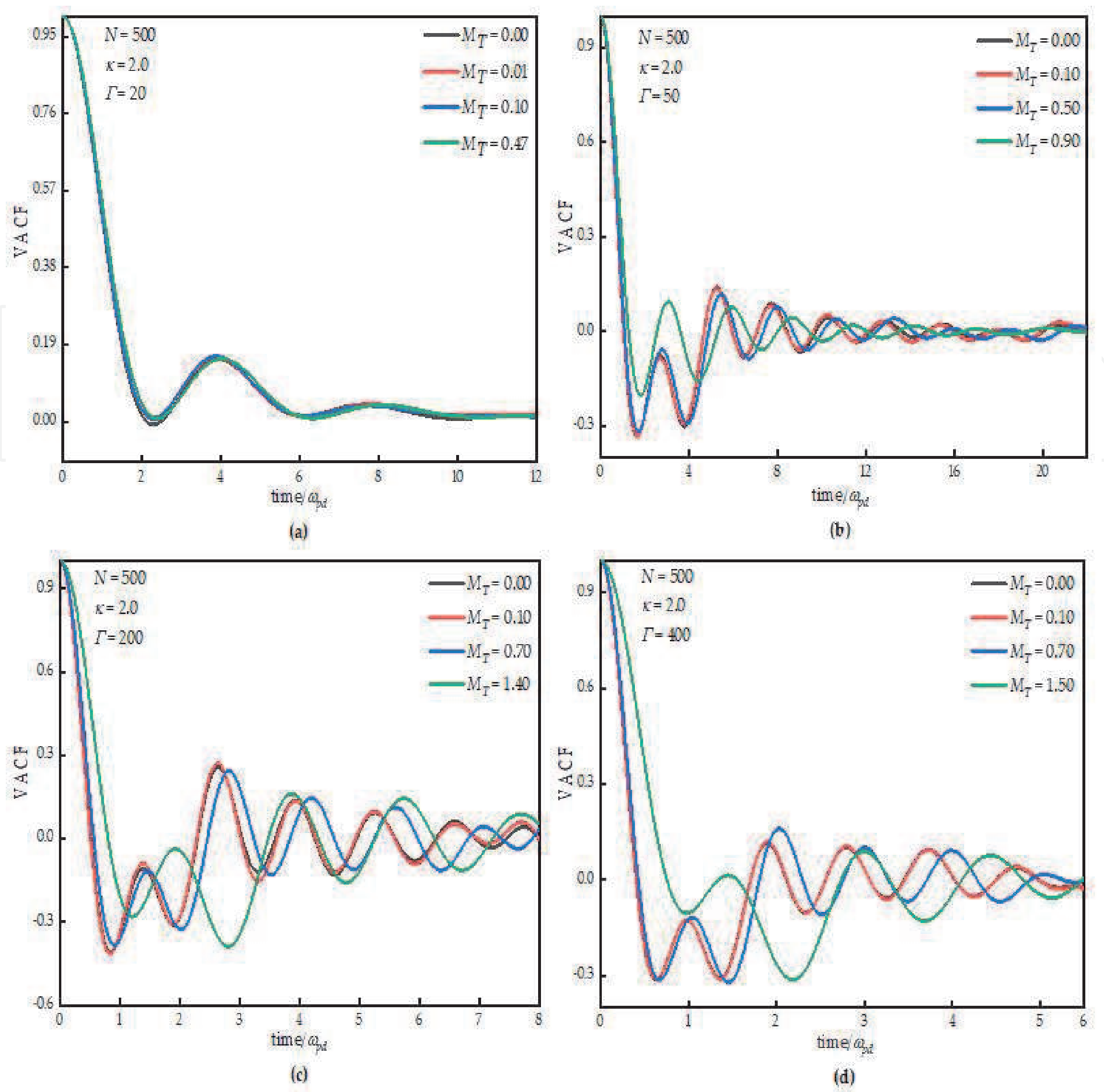

Figure 2.
VACF as a function of molecular dynamics simulation time scale for constant plasma screening parameter (κ = 2.0). MD simulations results obtained for N = 500 *simulated dust particles with the variation of uniaxial external electric field (0.0 <* $M_T \leq$ *1.30) and four different plasma regimes (a)* Γ = *20, (b)* Γ = *50, (c)* Γ = *200 and (d)* Γ = *400.*

for the same combinations of plasma parameters. It is noted that for plasma coupling (Γ = 20), the critical values (M_{CT} > 0.42) for κ = 1.4 display in **Figure 3**. We have found the increasing trend of M_T with increases the plasma coupling values or decreasing the system temperature such as Γ = 50, 100 and 200 critical $M_{CT} \geq$ 0.88, 1.12, 1.25 respectively. The possible reason for the low strength of M_T in high system temperature is the large interparticle distance show with the term ($1/\mathbf{r}^3$) in Eq. (1). The increasing values of D with respective of Γ at κ = 1.4 can be easily observed from four panels of **Figure 3**. Upon further increasing M_T, the MD simulation gives an error in the form of out of thermal equilibrium. At lower plasma coupling strength (Γ = 20), the D does not significantly increase under the applied external electric field's influence; only 0.03% observed the integral values of VACF. The increasing of diffusion was observed for Γ = 50 are 20%, Γ = 100 are 75% and Γ = 200 are 160%. The electric field effect on D in ER-CDPs can be found in the same as conventional electrorheological fluids and ionic liquids [40].

The simulation outcomes of D in 3D ER-CDPs at constant N = 500, different values of Γ as a function of the uniaxial electric field (M_T) for κ = 2 and 3 are shown in **Figures 4** and **5**, respectively. The effect of M_T was computed in four different

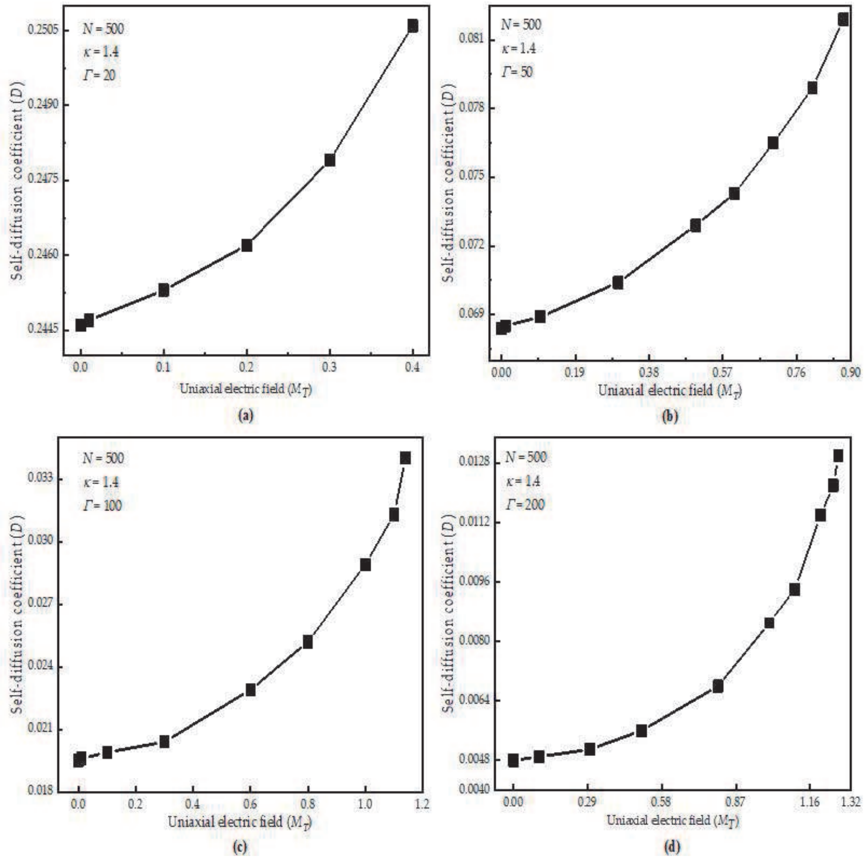

Figure 3.
Self-diffusion coefficient as a function of external applied uniaxial electric field (0.0 < M_T < 1.30), for constant plasma screening (κ = 1.4) and a number of particles (N = 500), considered four different ER-CDPs states (a) Γ = 20, (b) Γ = 50, (c) Γ = 100 and (d) Γ = 200.

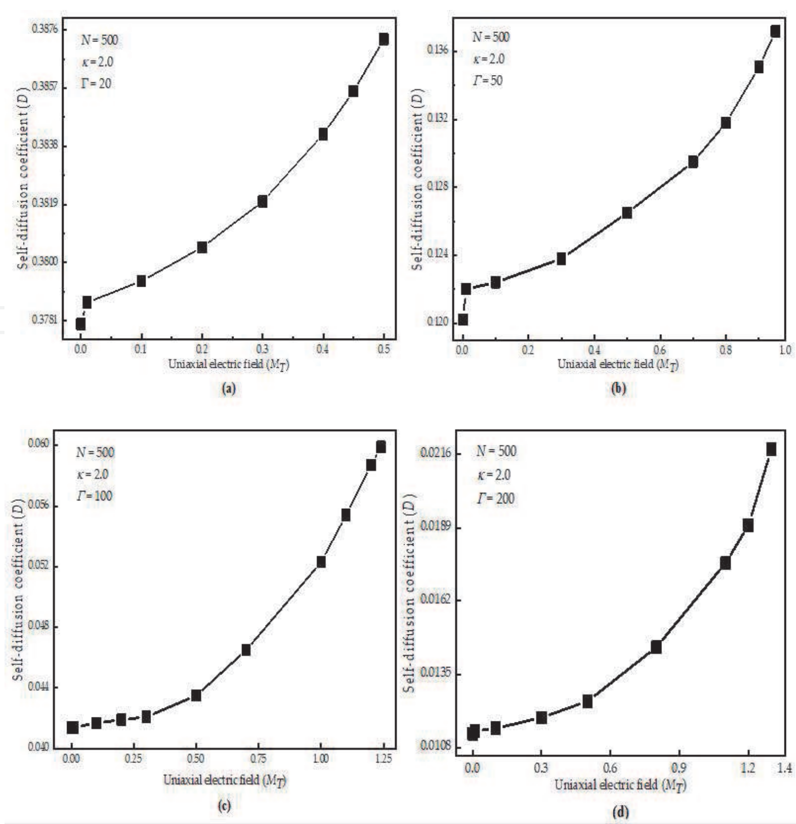

Figure 4.
Self-diffusion coefficient as a function of external applied uniaxial electric field (0.0 < M_T < 1.40), for constant plasma screening (κ = 2) and a number of particles (N = 500), considered four different ER-CDPs states (a) Γ = 20, (b) Γ = 50, (c) Γ = 100 and (d) Γ = 200.

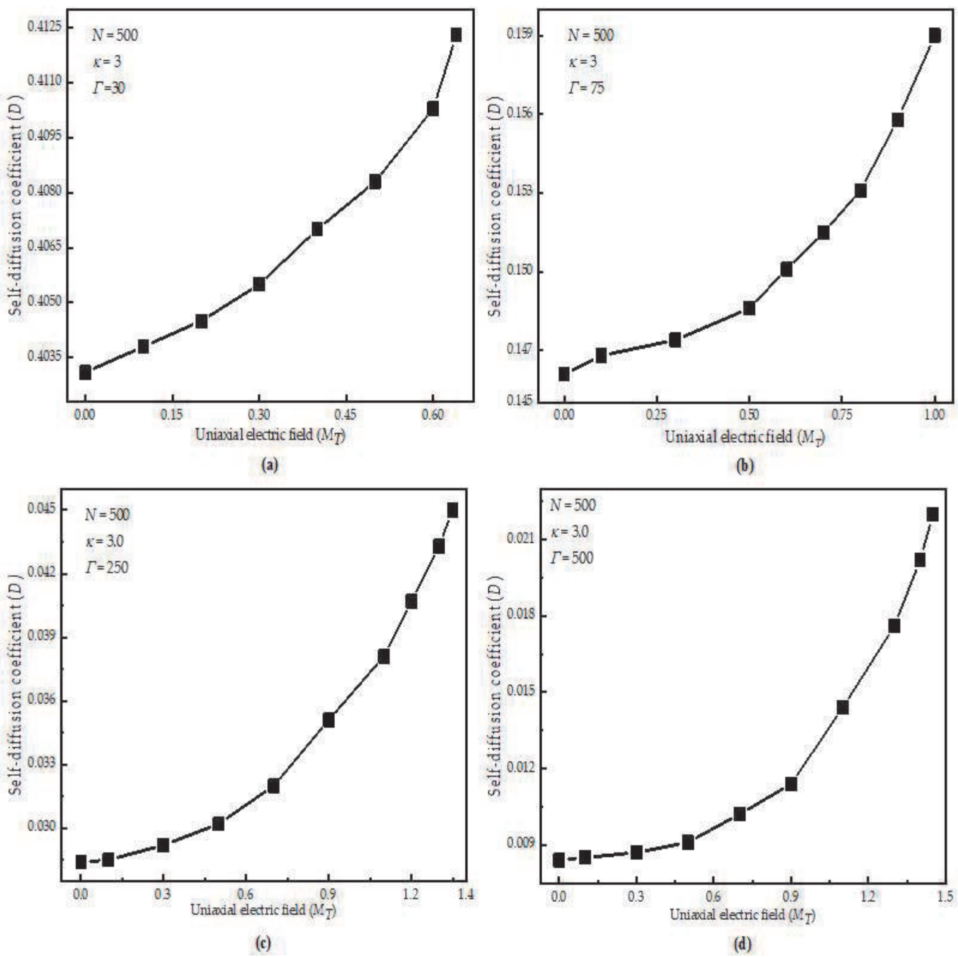

Figure 5.
Self-diffusion coefficient as a function of external applied uniaxial electric field ($0.0 < M_T < 1.50$), for constant plasma screening ($\kappa = 3$) and a number of particles ($N = 500$), considered four different ER-CDPs states (a) $\Gamma = 30$, (b) $\Gamma = 75$, (c) $\Gamma = 250$ and (d) $\Gamma = 500$.

states of ER-CDPs by performed almost thirty-three simulations. The M_{CT} values for $\kappa = 2.0$ at $\Gamma = 20$, $M_T > 0.45$, $\Gamma = 50$, $M_{CT} > 0.90$, $\Gamma = 100$, $M_{CT} > 1.23$, and $\Gamma = 200$, $M_{CT} > 1.35$. The increase in D under the action of external applied uniaxial electric field for $\Gamma = 20$, 50, 100, and 200 are 1.7, 11, 42, and 115%. The increases in the D for $\kappa = 3.0$ same N were observed nearly the same as said above for $\kappa = 2.0$. The effect of M_T on the D is prominent at higher values of Γ parameters. It was also noted that M_T does not significantly affect D lower to intermediate values of Γ. From **Figures 3–5**, we can conclude that the proposed MD simulation method worked for the limited strength of M_T. It was noted that the system's critical values above the system go out of thermal equilibrations, and kinetic energy increased very largely up to 23 orders of magnitude, but the potential energy does not change higher order of magnitude. Below the critical strength, the potential energy of interacting Yukawa dust particles increases with M_T.

4. Conclusion

An equilibrium MD simulation has been performed to report the velocity autocorrelation function (VACF) and self-diffusion coefficient (D) of three-dimensional (3D) electrorheological complex (dusty) plasmas (ER-CDPs) for the analysis of diffusion motion of dust particles. The interactions and forces between dust particles were modeled by Yukawa potential and Quadrupole interactions of charged dust particles. This paper highlights the outcomes of VACF and D for 3D

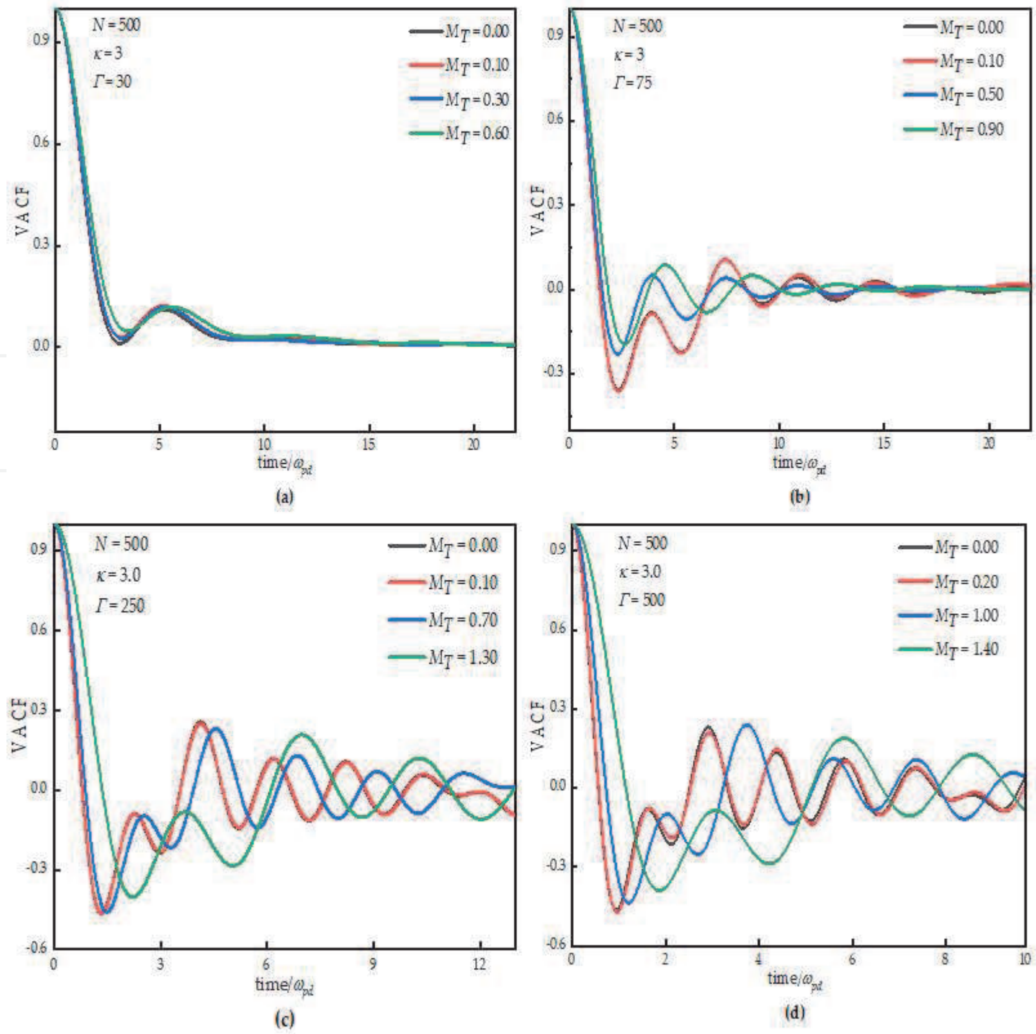

Figure 6.
VACF as a function of molecular dynamics simulation time scale for constant plasma screening parameter ($\kappa = 3.0$). *MD simulations results obtained for* N = 500 *simulated dust particles with the variation of uniaxial external electric field* ($0.0 < M_T \leq 1.30$) *and four different plasma regimes (a)* $\Gamma = 30$, *(b)* $\Gamma = 75$, *(c)* $\Gamma = 250$ *and (d)* $\Gamma = 500$.

ER-CDPs in the presence of a uniaxial electric field (M_T). We used Green-Kubo expression to calculate VACF and D over a wide range of CDPs Coulomb coupling (Γ) and Debye screening (κ) parameters. The VACF and D are significantly dependent on the plasma parameters (κ, Γ) and M_T. The calculated results are highly consistent with other MD data in the absence of M_T. It was observed that D decreased with increasing the Γ. The M_T significantly affects the diffusion motion in ER-CDPs from intermediate to higher values of Γ and does not affect low Γ. The D increases with increasing the M_T and κ. A new investigation gives more comprehensive and reliable data for VACF and D over given plasma parameters. It has been demonstrated that the presented numerical results for a given range of plasma parameters (Γ, κ) and the number of particles are good performances. The proposed numerical model is suitable for liquid-like and solid-like states for 3D CDPs. We can be concluded that the developed MD simulations approach will be employed to investigate the thermophysical properties of ER-CDPs.

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Abbreviation and symbol

EMD	Equilibrium molecular dynamic
ERFs	Electrorheological fluids
κ	Screening strength
Γ	Coulomb coupling
M_T	Thermal mach number
N	Number of particles
CDP	Complex (dusty) plasma
SCCDPs	Strongly coupled complex (dusty) plasmas
WCCDPs	Weakly coupled complex (dusty) plasmas
3D	Three dimensional
PK-3 plus	Plasma Kristall-3 plus
VACF	Velocity autocorrelation function
D	Self-diffusion coefficient
GKR	Green-Kubo relation
PBCs	Periodic boundary conditions
k_B	Boltzmann constant
ω_{pd}	Plasma frequency
T	Plasma temperature
a_{ws}	Wigner Seitz radius
θ	The angle between the electric field and particles vector

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