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NUMERICAL SIMULATION OF DUST PARTICLE IN WEAKLY IONIZED PLASMA IN COLLISIONAL REGIME WITH FINITE-DIFFERENCE LATTICE BOLTZMANN METHOD

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Summary. In this work, we present a numerical method for simulation of plasma around dust particle in collisional regime. It is based on finite-difference lattice Boltzmann method (FD-LBM) scheme which replaces Euler–Poisson equations for weakly ionized gas. It allows us to refine results obtained by means of drift-diffusion approximation due to the incorporation of convective term. The use of straightforward kinetic boundary conditions for perfect absorption allows us to calculate the non-zero concentration near the grain surface without any additional assumptions about flow structure, unlike other commonly used boundary conditions for full absorption. We demonstrate the capabilities of FD-LBM method to describe the process of dust grain charge and compare our results with some results of the numerical and analytic models of other authors.

1 INTRODUCTION

The problem of dust particle charging in collisional regime is of interest for complex plasma study [1]. Weakly ionized collisional plasma around dust grain is described with Euler–Poisson system. The quantitative study and the numerical approximation of the Euler–Poisson system is far from trivial, and usually charging process are considered with means of drift-diffusion approximation when one neglect convective term in Euler equation due to it smallness in comparison with drift and diffusion terms. One of the main advantages of such simplification is a possibility to obtain easily a numerical or even an analytic solution for grain charge, ion currents, floating potential and other parameters. Nevertheless, when convective term is not too small the drift-diffusion approximation leads to qualitatively correct but not very accurate results. In our opinion, one of the ways to solve Euler–Poisson system without physical simplifications is to use the kinetic approach to fluid dynamics. In the present work we study dust grain charging in collisional regime with the means of finite-difference lattice Boltzmann method (FD-LBM) [2, 3]. In this method the macroscopic equations (e.g. Euler, Navier–Stokes) are replaced with simplified kinetic equations, obtained from Boltzmann equation. The rest of the paper is organized as follows: in section 2 we outline mathematical model and in the section 3 we discuss our numerical solution and compare it with the solutions of other authors.

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2 FD-LBM MODEL

When we consider spherical dust grain charging in weakly ionized dense gas, we can describe this process with time dependent Euler–Poisson system of equations:

$$\frac{\partial}{\partial t}N_a + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 N_a V_a\right) = 0, \tag{1}$$

$$m_a N_a\left(\frac{\partial V_a}{\partial t} + V_a\frac{\partial V_a}{\partial r}\right) = -\frac{\partial}{\partial r}p_a - q_a N_a\frac{\partial \Phi}{\partial r} - \frac{\mu_{\text{an}} N_a V_a}{\tau_a}, \tag{2}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Phi}{\partial r}\right) = -\frac{1}{\varepsilon_0}\sum_a q_a N_a. \tag{3}$$

Here, r is the radial distance from the center of the grain, V_a the macroscopic velocity, N_a the density number and p_a the pressure of the charged species labeled with a (the subscripts $a = i$ and $a = e$ refer to ions and electrons, respectively). Φ is the electric potential, R the grain radius, and ε_0 the permittivity of vacuum. q_a and m_a are the charge and mass of particle a, respectively. Each species is assumed to obey the perfect gas equation of state $p_a = N_a k_B T$, where k_{B} is the Boltzmann constant. The quantities V_a, N_a, and Φ are functions of the r coordinate and time t. We assume frozen chemistry and the absence of neutral gas motions.

The last term on the right-hand side of equation (2) represents the drag force due to the collisions of charged particles with neutrals (ν_{an} is the frequency of collisions between neutral and charged particles and $\mu_{\text{an}} = m_a m_n/(m_a + m_n)$ is the reduced mass of charged particles with mass m_a and neutrals with mass m_n). The interparticle potential for the binary collisions between charged and neutral particles, is assumed inversely proportional to the fourth power of the separation distance. For this model, the collision frequencies are independent of the velocity of the charged particles [4].

System (1)–(3) is not easy to solve and mostly the process of grain charging are described by means of the drift-diffusion (DD) approximation. It could be derived by neglecting convective terms in Euler equation due to its smallness in comparison with drift and diffusion terms. Nevertheless, convective term could be significant near grain surface and using of drift-diffusion approximation could lead to quantitative errors. In our opinion, this problem could be solved using the kinetic representation of hydrodynamics. Kinetic-based methods, like LBM, allow obtaining the complete hydrodynamic solution (including convective term) without directly solving the system of hydrodynamic equation. Using the standard methodology [2, 3] we developed FD-LBM for system (1)–(3).

Essentially, as common for lattice Boltzmann methods we replace hydrodynamic equations with simplified kinetic equation for discrete distribution functions. This simplified kinetic equations for our method was derived from the continuous Boltzmann equation for the distribution

function F_a with a Bhatnagar–Gross–Krook-type (BGK-type) collision term for a spherically symmetric weakly ionized plasma flow [5]. In this paper we omit detailed derivation process (based on [2, 3]) and supply only governing FD-LBM system of simplified kinetic equations with the set of discrete velocities $\{c_j\}$ and BGK collision integral (complemented with Poisson equation). The dimensionless form of this system is:

$$\mathrm{St}_a \frac{\partial f_{a,j}}{\partial t} + \frac{c_j}{r^2}\frac{\partial}{\partial r}\left(r^2 f_{a,j}\right) = -\frac{f_{a,j} - f^0_{a,j}}{\mathrm{Kn}_a} - \left(\frac{1}{r} - \frac{Z_a}{2}\frac{\mathrm{d}\phi}{\mathrm{d}r}\right) G_{a,j}, \tag{4}$$

$$\frac{\varepsilon^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \varphi}{\partial r}\right) = -\sum_{a,j} Z_a f_{a,j}, \tag{5}$$

where G_i is the discrete representation of the force term. Here we use the following dimensionless variables

$$r \to \frac{r}{R},\ t \to \frac{t}{t_0},\ n_a = \frac{N_a}{N_0},\ u_a = \frac{V_a}{v_{\mathrm{Ta}}}, c = \frac{v_r}{v_{\mathrm{Ta}}}, \varphi = \frac{e\Phi}{k_{\mathrm{B}}T}, Z_a = \frac{q_a}{e},$$
$$\mathrm{St}_a = \frac{R}{v_{\mathrm{Ta}} t_0}, \mathrm{Kn}_a = \frac{v_{\mathrm{Ta}}}{\nu_{\mathrm{an}} R}, \tag{6}$$

where $v_{\mathrm{Ta}} = \sqrt{2k_{\mathrm{B}}T_a/m_a}$ is chosen as the reference velocity for a-component, R (grain radius) is the reference length and t_0 is reference time, St_a is Strouhal number, Kn_a is Knudsen number, $f_{a,j}$ is dimensionless discrete distribution function, $\varepsilon = \lambda_{\mathrm{D}}/R$, and $\lambda_{\mathrm{D}} = \sqrt{\varepsilon_0 k_B T/\left(N_0 e^2\right)}$ is the Debye screening length. Function $f^0_{a,j}$ is:

$$f^0_{a,j} = n_a w_j \left[1 - \left(\mu_a^2 + \frac{\mu_n^2}{3}\right) u_a^2 + 2\mu_a c_j u_a + \left(\mu_a^2 + \frac{\mu_n^2}{3}\right) c_j^2 u_a^2\right]. \tag{7}$$

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Dimensionless concentration and velocity of charged components are related to $f_{a,j}$ as:

$$n_a(r,t) = \sum_j f_{a,j}(r,t), \tag{8}$$

$$n_a(r,t)u_a(r,t) = \sum_j f_{a,j} c_j. \tag{9}$$

The set of discrete velocities (and its weights for (7)) is chosen to guarantee that 9 are corresponded to the solution of Euler equation in subsonic area:

$$c_1 = -\sqrt{3/2}\,, c_2 = 0, c_3 = \sqrt{3/2}\,, w_1 = 1/6,\ w_2 = 2/3,\ w_3 = 1/6. \tag{10}$$

The system of equations (4)–(5) is equivalent to the Euler–Poisson equations (1)–(3) in sub-

sonic areas, and allows us to obtain a solution of the problem within the framework of the kinetic theory instead of finding the solution of the Euler equations directly.

For the numerical integration we use IMEX scheme and convective term is approximated with WENO scheme. The resulting program code was tested and it successfully recreates different solutions of (1)–(3).

3 RESULTS AND DISCUSSION

As a kinetic method, FD-LBM is naturally applied for the time-dependent problems, such as dust grain charging. In this section, we demonstrate the capacity of the method for problem of dust grain charging in strong and fully collisional regime (using LBM for $\mathrm{Kn}[a] > 0.3$ requires significant modification of the method). In addition to aforementioned variables we also use the ion diffusion coefficient D_i and free mean path l_i. We consider spherical dust grain in weakly ionized gas without chemical reactions. The initial conditions in all computations are $n_a(r,0) = 1$, $u_a(r,0) = 0$, corresponding conditions for equation (4)

$$f_{a,1}(r,0) = \frac{1}{6},\ f_{a,2}(r,0) = \frac{2}{3},\ f_{a,3}(r,0) = \frac{1}{6}.$$

At outer border, $R_1 \gg R$, we use the equilibrium boundary condition in the equation (4):

$$f_{a,1}(R_1,t) = \frac{1}{6},\ f_{a,2}(R_1,t) = \frac{2}{3},\ f_{a,3}(R_1,t) = \frac{1}{6}.$$

The condition on the grain surface should describe the interaction of the gas particles with the surface. In this work we consider fully adsorbing particle ($c > 0$ correspond to particles flowing from surface), and in the continuous velocity space our boundary condition would be

$$f_a(c,R,t) = 0 \text{ if } c > 0. \tag{11}$$

The discrete analogue of (11) is

$$f_{a,3}(R,t) = 0. \tag{12}$$

We use the following boundary condition for the Poisson equation for the grain with charge Ze:

$$\varphi(R_1) = 0,\ \left.\frac{\mathrm{d}\varphi}{\mathrm{d}r}\right|_{r=R} = \frac{Z}{4\pi\varepsilon_0 R k_\mathrm{B} T}.$$

As the subject for numerical study, we choose a weakly-ionized gas mixture consisting of the buffer gas (Ar) under atmospheric pressure and the easily-ionized component (K). The temperature, concentrations, and grain radius are varied in different simulations.

The charge of the grain, immersed into plasma $Z(t)$ could be calculated at time t_1 as follows

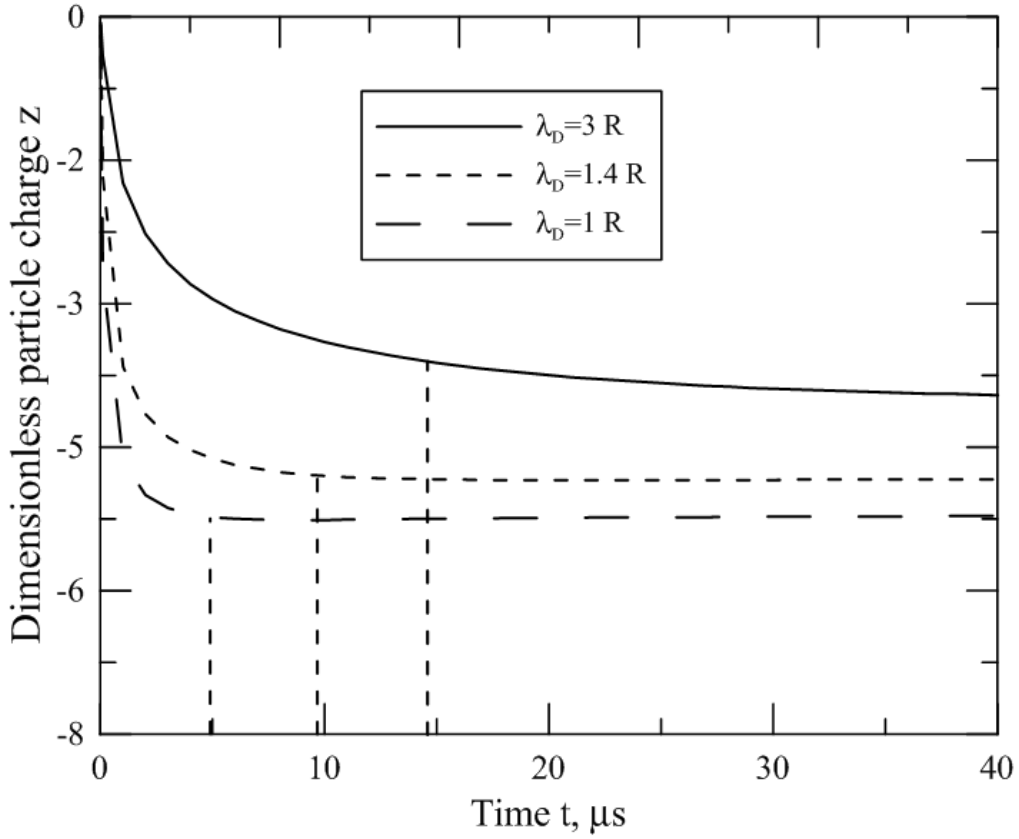


Figure 1: Grain charging in different regimes. Vertical lines mark charging time estimated in (14).

(assuming $Z(0) = 0$):

$$Z(t_1) = 4\pi R^2 \int_0^{t_1} (N_i(R,t)U_i(R,t) - N_e(R,t)U_e(R,t))\,\mathrm{d}t. \tag{13}$$

We expect that charging time in our calculations to agree with characteristic time scale t_Z [6] on which the dust particle reaches the steady state charge. It could be estimated as

$$t_Z \simeq \frac{d^2}{\pi^2 D_i}, \tag{14}$$

where d is the size of the non-quasineutral region. We can vary λ_D (and vary d with it) and see how the charging time in our calculations changes with it. For example if we fix all dimensional parameters except concentration and vary it so $\lambda_D = 3R$, $\lambda_D = 1.4R$ and $\lambda_D = 1R$ we estimate the charging time in (14) as 14 μs, 4 μs, 3 μs respectively for each concentration. Estimated charge time agrees well with the charging time in our calculation (figure 1) as expected.

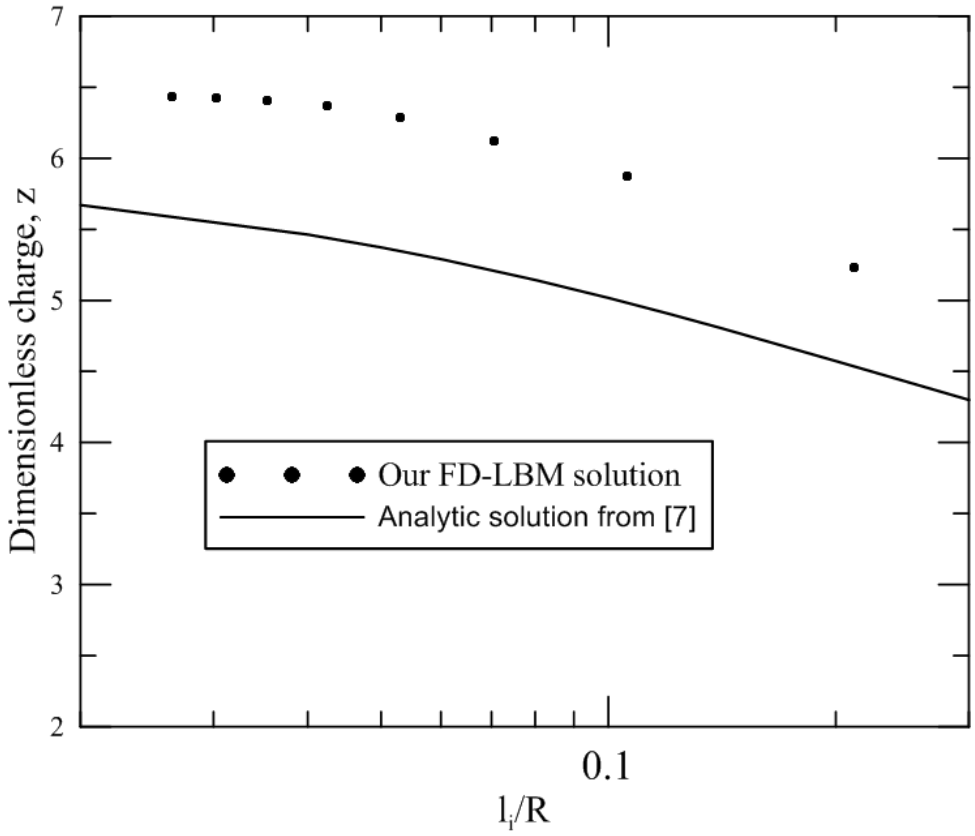
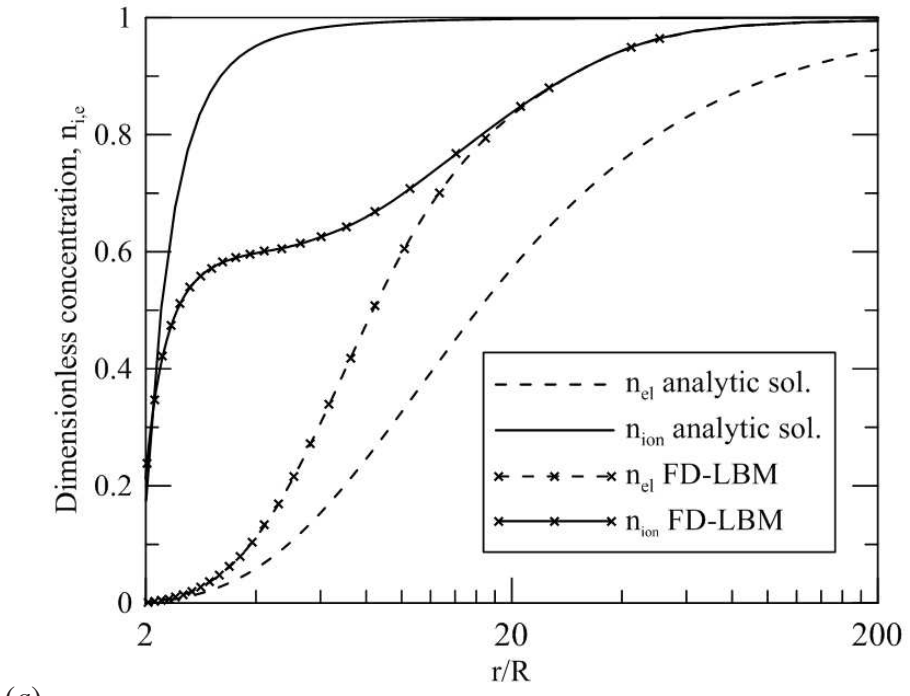
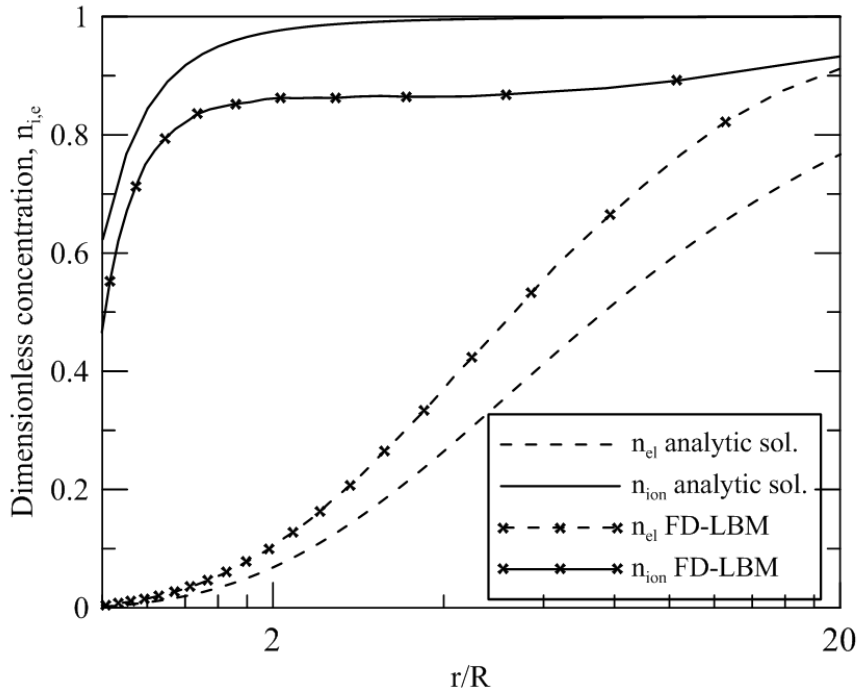


Figure 2: Dimensionless grain charge z as a function of the ion mean free path l_i normalized to the grain radius R for $\lambda_D = 2R$. Line—analytic solution from [7], dots—our numerical FD-LBM.

It is interesting to compare the results of our simulation with analytic solution for grain charge in collisional regime (drift-diffusion approximation). In [7] authors derive the analytic expression for dimensionless charge depending on Knudsen numbers $\mathrm{Kn}_{i,e}$ (in our notations) and ratio between ion and electron temperatures. Their model covers the wide range of regimes from fully collisional to OML and shows good comparison with experimental results in the weakly- and non-collisional areas ($\mathrm{Kn}_i > 10$), but it was derived under the condition $\lambda_D \gg R$. With our FD-LBM method we can compare this analytical solution with numerical solution when λ_D is of the same order as R. For example, in the case of $\lambda_D = 10R$ (fully collisional regime) the dimensionless charge z from our calculation and from [7] close to each other (4.8 and 5.1). But, for the case of $\lambda_D = 2R$ the differences between our numerical solution and analytical one is greater, see figure 2. Interesting to note that qualitatively z as the function of l_i/R in our calculation has the same form as in [7].



(*a*)



(*b*)

Figure 3: Dimensionless ion and electron concentration as a function of coordinate, normalized to the grain radius R; (*a*) $\lambda_D = 2R$, (*b*) $\lambda_D = 10R$.

In [7] there is also analytic solution for electron and ion charged density in the hydrodynamic regime, let us compare it with our results. In [7] authors operate under condition $\lambda_D \gg R$, but it is interesting to see how close to our numerical solution their results are when λ_D close to R. We expect good matching near grain, where electric field is not screened. For this comparison we consider fully and strong collisional regimes only, as regimes with $\mathrm{Kn} > 0.1$ demand significant alterations of LBM. Figure 3 demonstrates dimensionless concentration of ions and electrons for two cases—$\lambda_D = 2R$ and $\lambda_D = 10R$. As we expected, analytic formula for concentration from [7] work more or less correctly near grain even if condition $R \ll \lambda_D$ is violated.

Near grain we mostly attribute the difference in solution to the errors of drift-diffusion approximation. We can calculate the relation between convection and drift-diffusion terms in our calculations. Let us call it α:

$$\alpha = \left| \frac{n_a u_a \frac{\partial u_a}{\partial r}}{-\frac{Z_a n_a}{2} \frac{d\phi}{dr} - \frac{1}{2} \frac{\partial n_a}{\partial r}} \right|. \tag{15}$$

When $\alpha \ll 1$ it is safe to use DD approximation, otherwise it could lead to numerical errors. For the calculations above typical α is between 0.2 and 0.4, so one should not neglect convective term for precise calculation. For example, if we look at the results from [8], where authors consider grain charge on the basis of Vlasov-BGK equations, we can see that our concentrations from figure 3 ($\lambda_D = 2R$ and $\lambda_D = 10R$) are close to the solutions of [8] in the fully collisional regime (the comparisson is valid due to very small temperature change in collisional regime in [8]). And while Vlasov equation allows to obtain solution for high Kn_a too, it is far more complicated and require more time for numerical solution than kinetic equations of LBM method.

4 CONCLUSIONS

The proposed kinetic model allows us to obtain the solution for an isothermal Euler–Poisson system of a weakly ionized gas around the dust particle. It works well in collisional regimes, reproduces some analytic and numerical solutions, and refines the drift-diffusion approximation. We show that incorporating of the convective term (as opposed to the drift-diffusion approximation) could change the concentration and flow in the region near the grain.

The use of straightforward kinetic boundary conditions for perfect absorption allows us to calculate the non-zero concentration near the grain surface without any additional assumptions about flow structure, unlike other commonly used boundary conditions for full absorption.

In summary, the discrete kinetic model derived from the Boltzmann equation seemed to be a reasonable compromise between physical accuracy and computational effort. Future research will be aimed at the elimination of errors related to the significant value of the macroscopic velocity and at solving the thermal Euler–Poisson equations.

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REFERENCES

[1] V. E. Fortov and G. E. Morfill, *Complex and Dusty Plasmas: From Laboratory to Space*, Series in Plasma Physics (CRC Press, Boca Raton, FL, 2010).
[2] X. He and L. S. Luo, *Phys. Rev. E* **55**, R6333 (1997).
[3] X. Shan, X. F. Yuan, and H. Chen, *J. Fluid Mech.* **550**, 413 (2006).
[4] T. Kihara, M. H. Taylor, and J. O. Hirschfelder, *Phys. Fluids* **3**, 715 (1960).
[5] Y. S. Chou, L. Talbot, and D. R. Willis, *Phys. Fluids* **9**, 2150 (1966).
[6] A. F. Pal', A. N. Starostin, and A. V. Filippov, *Plasma Phys. Rep.* **27**, 143 (2001).
[7] L. G. D'yachkov, A. G. Khrapak, S. A. Khrapak, and G. E. Morfill, *Phys. Plasmas* **14**, 042102 (2007).
[8] I. L. Semenov, A. G. Zagorodny, and I. V. Krivtsun, *Phys. Plasmas* **18**, 103707 (2011).

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