NUMERICAL STUDY OF GRAIN CHARGING KINETICS ON THE BASIS OF BGK KINETIC EQUATION

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An investigation of charging a spherical particle in partially ionized nonisothermal plasma is carried out on the basis of the numerical solution of the BGK (Bhatnagar–Gross–Krook) model kinetic equation. Stationary values of the particle charge and the electron and ion currents are calculated for various collisional regimes. It is verified that, for the strongly collisional regime, the effective potential has a Coulomb form at large distance from the particle surface. A new BGK-type model for binary gas mixtures is proposed. It is shown that this model satisfies all the basic properties of Boltzmann collision integrals including the correct exchange coefficients. A high-order implicit numerical method for solving the kinetic equations is developed. The method is conservative with respect to the collision integrals for arbitrary values of the Knudsen number.

1. Introduction

Studying the grain charging and screening in a plasma background is an important problem in dusty plasma physics. The process of grain charging is governed by ion and electron currents. For typical plasma parameters that are recorded in experiments on dusty plasmas, the collisions between charged particles can be neglected. Consequently, the ion and electron fluxes to the grain surface are influenced mainly by electron-neutral and ion-neutral collisions. The frequency of these collisions depends on the density of neutrals. The grain charging in a weakly collisional background is considered in many works, e.g., [1, 2]. The opposite limit of a strongly collisional background is investigated in [3] on the basis of a drift-diffusion approach. In addition, the ion velocity distribution and the ion current on a particle in plasma are calculated in [4, 5] on the basis of the BGK model kinetic equation for ions.

The aim of this work is to study the charging and the screening of a spherical grain in all collisional regimes, including the transient one. In this regime, the electron-neutral and ion-neutral mean free paths are comparable with the Debye length. The charging process is investigated on the basis of kinetic equations for ions and electrons in the sphericaly symmetric case. Boltzmann collision integrals in these equations are replaced with BGK-type model collision integrals that satisfy all basic properties: conservation laws, correct equilibrium state, entropy inequality, and correct exchange coefficients. The last property is crucial for particles with different masses (e.g., electron-neutral systems). The kinetic equations are solved numerically by means of a high-resolution implicit conservative scheme that is described below in detail. For simplicity, He is considered as the example of a plasma background. In all computations, the plasma background temperature equals $T_0 = 0.1$ eV, plasma background density equals $n_e^0 = n_i^0 = 10^{10}$ cm^{-3}, electron-neutral collision cross section equals $\sigma_{en} = 5 \times 10^{-16}$ cm^2, ion-neutral collision cross-section equals $\sigma_{in} = 27.9 \times 10^{-16}$ cm^2 (charge exchange cross section), and grain radius equals $r_0 = 10^{-2}$ cm. The density of background neutrals varies in the range $n_n^0 = 10^{15} \div 10^{18}$ cm^{-3}.

2. Basic Equations

As mentioned above, we consider only two types of plasma particles: ions and electrons. Moreover, let us consider, for simplicity, only singly ionized ions. In view of a low density of charged particles, we can neglect collisions between them and assume that electron-neutral and ion-neutral collisions do not change a state of neutrals. Hence, let us consider the kinetic equations for ions and electrons with regard for the spherical symmetry. In this case, the distribution functions for ions f_i and electrons f_e depend on time $t \geq 0$, radius $r > 0$, radial velocity $-\infty < \xi_r < \infty$, and absolute value of angular velocity $\xi = \sqrt{\xi_\varphi^2 + \xi_\theta^2} \geq 0$, where ξ_φ and ξ_θ are components of the angular velocity. The kinetic equations have form

$$\frac{\partial f_e}{\partial t} + \xi_r \frac{\partial f_e}{\partial r} + \left(\frac{\xi^2}{r} - \frac{eE}{m_e}\right)\frac{\partial f_e}{\partial \xi_r} - \frac{\xi_r \xi}{r}\frac{\partial f_e}{\partial \xi} = J_{en}, \quad (1)$$

$$\frac{\partial f_i}{\partial t} + \xi_r \frac{\partial f_i}{\partial r} + \left(\frac{\xi^2}{r} + \frac{eE}{m_i}\right)\frac{\partial f_i}{\partial \xi_r} - \frac{\xi_r \xi}{r}\frac{\partial f_i}{\partial \xi} = J_{in}, \quad (2)$$

where J_{en} and J_{in} are electron-neutral and ion-neutral collision integrals, respectively. The equation for the self-consistent electric field E reads as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 E\right) = \frac{e}{\varepsilon_0}\left(n_i - n_e\right), \quad (3)$$

where n_e and n_i are the electron and ion densities, respectively. The grain charge emerges due to a difference between the electron and ion mobilities. The equation for the grain charge can be written as follows:

$$\frac{dQ_g}{dt} = -4\pi r_0^2 e\left(n_i u_i - n_e u_e\right)_{r=r_0}, \quad (4)$$

where Q_g is the grain charge, and u_e, u_i are electron and ion velocities, respectively. The electron and ion macroscopic parameters (density, velocity, temperature, *etc.*) at each value of radius r are calculated as the moments of the distribution functions f_e and f_i:

$$n_\alpha = 2\pi \int_{-\infty}^{\infty}\int_0^{\infty} f_\alpha\, \xi\; d\xi_r d\xi, \quad (5)$$

$$u_\alpha = \frac{2\pi}{n_\alpha} \int_{-\infty}^{\infty}\int_0^{\infty} \xi_r f_\alpha\, \xi\, d\xi_r d\xi, \quad (6)$$

$$T_\alpha = \frac{2\pi}{3kn_\alpha} \int_{-\infty}^{\infty}\int_0^{\infty} m_\alpha\left(\xi_r - u_\alpha\right)^2 f_\alpha\, \xi\, d\xi_r d\xi, \quad (7)$$

where $\alpha = e, i$, and T_α is the temperature of charged particles.

The problem for Eqs. (1)–(4) is considered in the domain $r_0 \leq r \leq R$, $t \geq 0$. It is assumed here that the point $r = 0$ coincides with the grain center, and a value of R is large enough to suppose that plasma at this boundary is undisturbed. At the left boundary (on the grain surface) $r = r_0$, the following boundary condition is used:

$$f_e = 0\,, f_i = 0,\ \xi_r \geq 0;\ E = Q_g/(4\pi\varepsilon_0 r_0^2). \quad (8)$$

It should be noted that the distribution functions for falling particles at this boundary, i.e., for $\xi_r < 0$, are obtained from the solution of Eqs. (1)–(2) in accordance with the classical problem statement for the Boltzmann equation. Thus, the ion and electron fluxes on the grain surface, i.e., at the point $r = r_0$, in Eq. (4) are calculated with the use of Eqs. (5) and (6).

At the right boundary $r = R$, the undisturbed background distribution functions are maintained:

$$f_e^0 = n_e^0\left(\frac{m_e}{2\pi kT_0}\right)^{3/2}\exp\left(-\frac{m_e(\xi_r^2 + \xi^2)}{2kT_0}\right), \quad (9)$$

$$f_i^0 = n_i^0\left(\frac{m_i}{2\pi kT_0}\right)^{3/2}\exp\left(-\frac{m_i(\xi_r^2 + \xi^2)}{2kT_0}\right), \quad (10)$$

where $\xi_r \leq 0$. Here again, the distribution functions for $\xi_r > 0$ are obtained by solving Eqs. (1)–(2).

For the initial moment $t = 0$, we assume that the relations $f_i = f_i^0$, $f_e = f_e^0$, and $Q_g = 0$ hold. In the present work, we are mainly interested in the steady-state solution of Eqs. (1)–(4). In that case, the final steady-state value of the grain charge is obtained as the steady-state solution of Eq. (4), the final radial distributions of ion and electron macroscopic parameters are obtained from the steady-state solution of Eqs. (1)–(2) and (5)–(7), and the final radial distribution of the electric field is obtained from (3).

3. Model Collision Integrals

Further, let us consider the BGK-type model collision integrals J_{en} and J_{in}. For brevity, only electron-neutral systems are considered. Thus, the electron-neutral model collision integral reads as

$$J_{en} = \omega_e\left(M_e^1 - f_e\right) + \omega_e\frac{4\mu_{en}}{(m_e + m_n)}\left(M_e^2 - f_e\right), \quad (11)$$

where $\omega_e = \nu_1 n_n$, μ_{en} is the reduced electron-neutral mass, n_n is the density of neutrals, and the coefficient ν_1 characterizes the electron-neutral collision frequency. The functions M_e^1 and M_e^2 are as follows:

$$M_e^1 = n_e \left(\frac{m_e}{2\pi k\hat{T}_e}\right)^{3/2} \exp\left(-\frac{m_e(c_{en}^2+\xi^2)}{2k\hat{T}_e}\right), \quad (12)$$

$$M_e^2 = n_e \left(\frac{m_e}{2\pi k\hat{T}_{en}}\right)^{3/2} \exp\left(-\frac{m_e(c_e^2+\xi^2)}{2k\hat{T}_{en}}\right), \quad (13)$$

where $c_{en} = \xi_r - u_{en}$, $c_e = \xi_r - u_e$,

$$u_{en} = \frac{m_e u_e + m_n u_n}{m_e + m_n},$$

$$\hat{T}_{en} = \frac{T_e + T_n}{2},$$

$$3k\hat{T}_e = 3kT_e + m_e(u_e - u_{en})^2,$$

and u_n is the velocity of neutrals. It can be shown that if the neutral-electron collision integral J_{ne} is also written in the form (11), then the model collision integrals J_{en} and J_{ne} satisfy all basic properties (conservation laws, entropy inequality, correct equilibrium state) of Boltzmann collision integrals. In addition, the proposed form of model integrals provides a correct expression for its first moments, i.e., the correct exchange coefficients are achieved.

4. Numerical Method

The equations (1)-(4) are solved numerically in dimensionless form. The following dimensionless variables are used for electrons: $\tilde{r} = r/r_0$, $\tilde{t} = t\,r_0/v_e$, $\tilde{n}_e = n_e/n_e^0$, $\tilde{T}_e = T_e/T_0$, $\tilde{\xi}_r = \xi_r/v_e$, $\tilde{\xi} = \xi/v_e$, $\tilde{u}_e = u_e/v_e$, $\tilde{f}_e = f_e\, v_e^3/n_e^0$, where $v_e = \sqrt{2kT_0/m_e}$. For ions, we use the dimensionless variables $\tilde{r} = r/r_0$, $\tilde{t} = t\,r_0/v_i$, $\tilde{n}_i = n_i/n_i^0$, $\tilde{T}_i = T_i/T_0$, $\tilde{\xi}_r = \xi_r/v_i$, $\tilde{\xi} = \xi/v_i$, $\tilde{u}_i = u_i/v_i$, $\tilde{f}_i = f_i\, v_i^3/n_i^0$, where $v_i = \sqrt{2kT_0/m_i}$. The dimensionless electric field is $\tilde{E} = E\,(er_0/2kT_0)$, and the dimensionless grain charge is $\tilde{Q}_g = Q_g/(4\pi r_0^3 n_e^0 e)$. The final dimensionless form of the basic equations is omitted for brevity, but it should be noted that, in the final form, these equations contain three basic dimensionless parameters: r_D – non-dimensional Debye length, K_{en} – electron-neutral Knudsen number, and K_{in} – ion-neutral Knudsen number that have the form

$$r_D = \frac{1}{r_0}\sqrt{\frac{2kT_0\varepsilon_0}{e^2 n_e^0}},$$

$$K_{en} = v_e \tau_{en}/r_0,$$

$$K_{in} = v_i \tau_{in}/r_0.$$

The electron-neutral collision frequency is defined as $\tau_{en}^{-1} = n_n^0\sqrt{2E_H/m_e}\ \sigma_{en}$, and the ion-neutral collision frequency is defined as $\tau_{in}^{-1} = n_n^0(4/3)\sqrt{8kT_0/\pi\mu_{in}}\ \sigma_{in}$, where μ_{in} is the ion-neutral reduced mass.

In order to digitize the kinetic equations (1), (2) and Eq. (3) we introduce a conventional finite-volume mesh in the physical and velocity spaces. At that, the mesh in the velocity space is uniform, and the radial mesh is nonuniform with clustering at the grain surface. For the time digitization of Eqs. (1) and (2), the implicit factored scheme [6] is used. Spatial derivatives are approximated by means of the 5-th order finite-volume WENO scheme [7]. Ion and electron macroscopic parameters are calculated from Eqs. (5)-(7) by means of the second-order central point quadrature rule. In order to make the method conservative with respect to the collision integrals for arbitrary values of the Knudsen numbers, the correction procedure proposed in [8, 9] is used. Equation (4) for the grain charge is solved by the one-step explicit Euler method, and the electric field is obtained from the integral form of Eq. (3) (by means of the Ostrogradskii–Gauss theorem):

$$E(r) = \frac{Q(r)}{4\pi r^2 \epsilon_0}, \quad (14)$$

where $r_0 \le r \le R$, and

$$Q(r) = Q_g + 4\pi \int_{r_0}^{r} e\,(n_i - n_e)\ r^2 dr \quad (15)$$

is the total charge within a sphere with radius r. The integral in (15) is calculated by means of the composed trapezoidal method. In all computations, we took $R = 50r_D$, where R is given in dimensionless form.

5. Numerical Results

Let us consider the results obtained from the numerical solution of Eqs. (1)–(4). In all computations, the dimensionless Debye length equals $r_D = 0.33$, and the approximate equality $K_{en} \approx K_{in}$ holds. Figure 1 illustrates the final steady-state relative charge distributions $Q(r)/Q_g$ for various Knudsen numbers. Here, $Q(r)$ is calculated with the help of Eq. (15), and Q_g is the steady-state solution of Eq. (4). The density, velocity, and temperature radial distributions for various Knudsen numbers

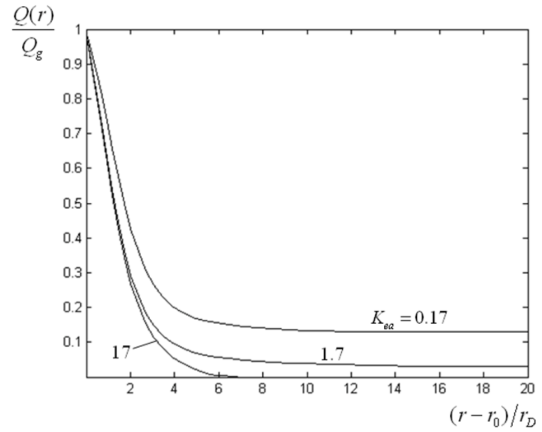

Fig. 1. Relative charge distribution for various Knudsen numbers

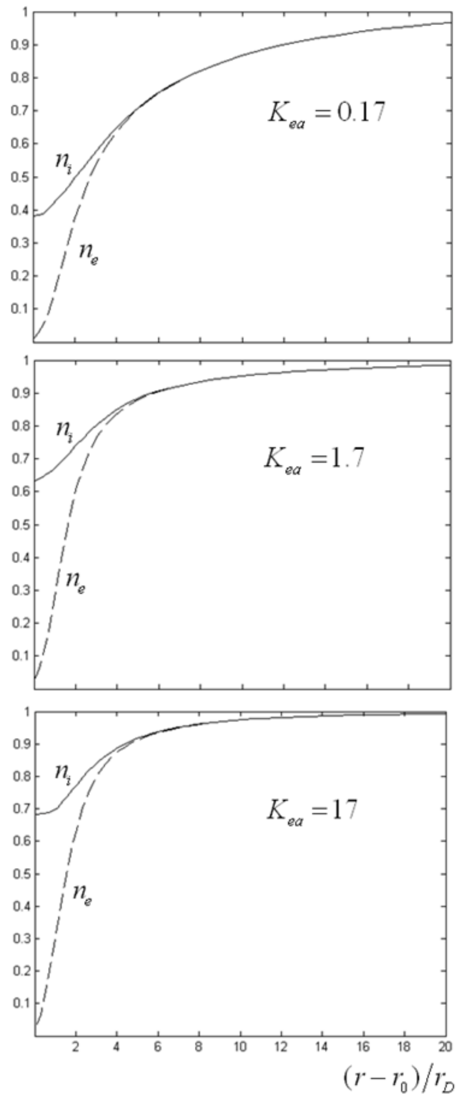

Fig. 2. Density distribution for various Knudsen numbers

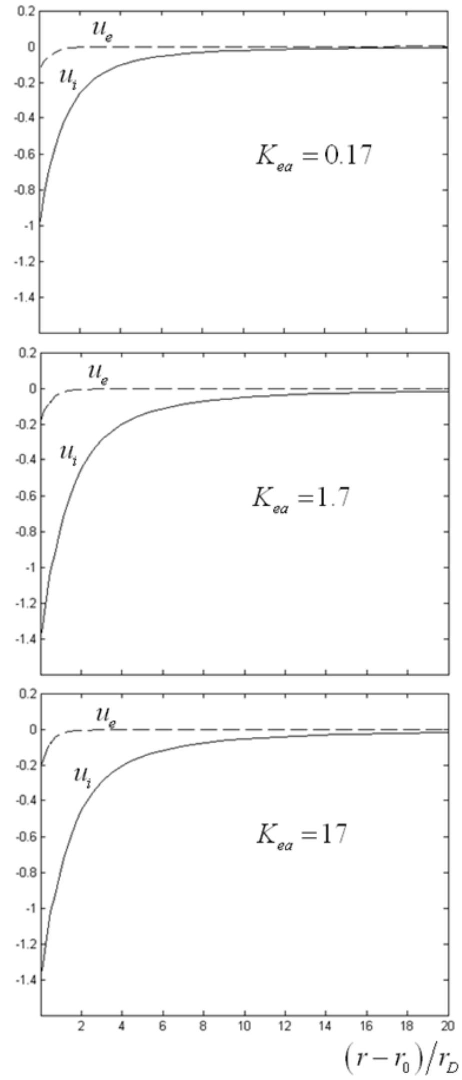

Fig. 3. Velocity distribution for various Knudsen numbers

in the final steady-state regime are shown on Figs. 2-4, respectively. It should be noted that all values presented in these figures are obtained for dimensionless variables. Thus, we refer the reader to the beginning of Section 4 for more details.

One can see from Fig. 2 that there exists a sheath near the grain surface that ranges up to $10r_D$. For the strongly collisional regime where $K_{ea} \ll 10r_D$, we observe the Coulomb-type asymptotic behavior of the screened field with some effective charge (see Fig. 1, $K_{ea} = 0.17$). This result correlates with that of [3]. In the opposite limit of a collisionless sheath where $K_{ea} \gg 10r_D$, we observe a finite screening length (see Fig. 1, $K_{en} = 17$). This result is also in agreement with analogous calculations [1, 2]. For the transient regime

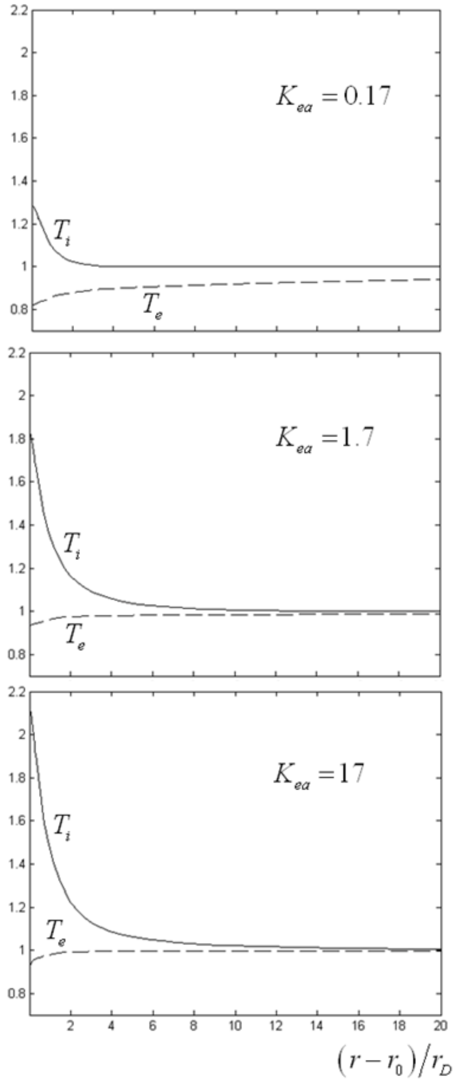

Fig. 4. Temperature distribution for various Knudsen numbers

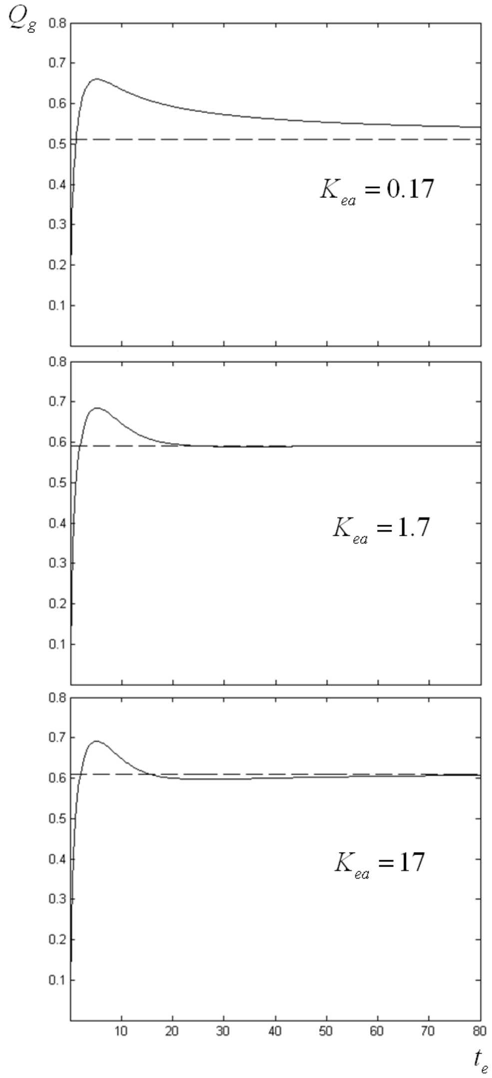

Fig. 5. Grain charging kinetics for various Knudsen numbers. Dotted line shows the stationary value of the grain charge

where the sheath is weakly collisional, we also observe the Coulomb-type asymptotic behavior of the screened field (see Fig. 1, $K_{en} = 1.7$). But, in this case, the value of effective charge is smaller than that for the strongly collisional regime.

Finally, Fig. 5 demonstrates the grain charging kinetics for various Knudsen numbers. Here, the grain charge Q_g is measured in $4\pi r_0^3 n_e^0 e$, and the time t_e is measured in r_0/v_e (see Section 4). The dotted line in this figure represents a stationary value of the grain charge. One can see from Fig. 5 that the stationary value of the grain charge decreases with decrease in the Knudsen number. In addition, one can observe a nonmonotonic behaviour of the charging curve. As shown in Fig. 5, the grain charging is a two-stage process. The first stage is relatively short. Its duration is approximately $10r_0/v_e$, and this stage corresponds to the establishment of the electron flow. The second stage is longer than the first one. It corresponds to the establishment of the ion flow, and its duration increases with decrease in the Knudsen number. Hence, the total duration of the establishment of the steady-state regime depends mainly on the duration of the second stage of the charging process.

6. Conclusions

In the present work, the grain charging kinetics is investigated numerically on the basis of model kinetic equa-

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tions for ions and electrons. A new BGK-type model for binary gas mixtures is proposed. It is shown that this model satisfies all the basic properties of Boltzmann collision integrals including correct exchange coefficients. A high-order conservative implicit numerical method for solving the kinetic equations is developed.

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ЧИСЕЛЬНЕ ДОСЛІДЖЕННЯ КІНЕТИКИ ЗАРЯДЖАННЯ ЧАСТИНКИ НА ОСНОВІ КІНЕТИЧНОГО РІВНЯННЯ БАТНАГАРА–ГРОССА–КРУКА

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Р е з ю м е

Проведено дослідження заряджання сферичної частинки в частково іонізованій неізотермічній плазмі на основі чисельного розв'язку модельного кінетичного рівняння Батнагара–Гросса–Крука. Визначено стаціонарні значення заряда частинки, електронного та іонного струмів для різних режимів зіткнень. Показано, що в континуальному режимі ефективний потенціал має кулонівський вигляд на великих відстанях від частинки. Запропоновано нову модель БГК типу для бінарної суміші газів. Показано, що дана модель задовольняє основні властивості інтегралів зіткнень Больцмана, включаючи коректні рівняння переносу. Розроблено неявну схему високого порядку точності для розв'язку кінетичного рівняння. Показано, що метод є кінетично консервативним при довільних значеннях числа Кнудсена.