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Author(s)	Kobayashi, Tsukasa; Sugawara, Hirotake; Ikeda, Kei
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An improved calculation scheme of electron flow in propagator method for solving the Boltzmann equation

Tsukasa Kobayashi^{1*}, Hirotake Sugawara², and Kei Ikeda¹

¹*ATHENASYS Co., Ltd., Kugenuma-Kaigan 3-3-4, Fujisawa, Kanagawa 251-0037, Japan*

²*Graduate School of Information Science and Technology, Hokkaido University, Sapporo 060-0814, Japan*

In order to accurately evaluate the electron acceleration process in the time evolution calculation of electron velocity distribution function (EVDF) based on the Boltzmann equation, an improved scheme blending upwind and central differences is introduced into the propagator method (PM). While the previous PM based on the upwind scheme needs fine cells to obtain an accurate EVDF at low electric fields, the improved PM is robust against coarse cells, which allows the reduction of the cell resolution. Calculations of the EVDF in Ar under RF electric fields demonstrated that the blending scheme can provide satisfactorily accurate results even with cells about tenfold larger than the upwind case at low reduced electric fields below 1 Td, which leads to much shorter computational time because the reduction of number of cells satisfactorily compensates the complexity of the blending scheme. This technique has been built into a new user-friendly PM software named BOSPROM.

1. Introduction

Several different approaches are known for simulating nonequilibrium low-temperature plasmas.¹⁾ In general, particle-based plasma simulations are characterized by high accuracy in reproducing kinetic phenomena, but they are not practical enough for engineering applications because they require enormous computation time. On the other hand, plasma simulations based on fluid models, although they are not highly accurate, are widely used because reasonably accurate results can be obtained in a short time and there are several general-purpose software packages available.²⁻⁵⁾ In the plasma fluid model simulation, data of transport coefficients and reaction rate constants of chemical species, i.e., swarm parameters, are required as prerequisites. For electrons, on the basis of electron velocity distribution function (EVDF) calculated by the Boltzmann equation (BE) analysis, the relationship between electron temperature and swarm parameters has been provided as a lookup table, which is referred to during the calculation of the fluid model. The basic equation of the BE analysis is the BE

*E-mail: tks@athenasys.co.jp

simplified under the spatially uniform condition, and the data of the electron collision cross section is required as input data for the analysis. In most cases, the EVDF in a real gas significantly deviates from a Maxwellian. On the other hand, the basic equations of the fluid model of plasma are simplifications of the original BE assuming that the EVDF is close to a Maxwellian. Therefore, there is no physical justification for applying the solution of BE analysis to the fluid model. The treatment of swarm parameters in fluid models is regarded as a kind of patch technique. Nevertheless, the method is empirically known to yield good results, and is widely used for its convenience in numerous studies and applications (only several examples are cited as references).^{6–10)} In the general plasma fluid models, swarm parameters obtained by BE analysis under DC electric fields have been usually used even for the simulation of RF plasmas. As another option, it is possible to use the swarm parameters obtained by BE analysis under RF electric fields. From a practical viewpoint, it is interesting what results are yielded by the swarm parameters obtained under RF electric fields.

The most commonly used method of BE analysis is the two-term approximation,^{1,11)} where the BE is solved by approximating the EVDF as the sum of only two components: isotropic one and anisotropic one proportional to $\cos \theta$ (θ is the angle between the electron velocity and the acceleration direction). The free software BOLSIG+¹²⁾ is very well known and widely used for many fluid model simulations. Similar software LoKI-B¹³⁾ has also been developed. However, BOLSIG+ has the following drawbacks: the calculation is unstable for strongly electronegative gases, the frequency of AC electric fields is limited to the microwave range or higher, and the approximation accuracy is insufficient under strong electric fields. The multi-term approximation is a solution method for the BE that further improves the approximation accuracy, and it has been reported that about 6 terms are required in CH₄ gas.¹⁴⁾ There is an open-source software MultiBolt.¹⁵⁾ Although several different advanced methods are known as exact solution methods for the BE, the most well-known one is Monte Carlo method (MC).^{1,16)} Some programs such as METHES¹⁷⁾ and LoKI-MC.¹⁸⁾ are known. In this method, the time evolution of EVDF is calculated on the basis of the motion of a finite number of representative electrons which is stochastically tracked using random numbers to determine the electron free flight time or to judge the occurrence of a collisional event, and the final steady-state EVDF is obtained. However, in order to reduce the statistical fluctuation, it is necessary to sample a large number of representative electrons. Because of the high computational cost (it increases further in the case under RF electric fields), the MC results were rarely applied to data preparation for fluid model.

Up to now, one of the most promising exact solution techniques for BE is the propagator

method (PM).¹⁹⁾ The PM is different from MC, though both methods track the time evolution of EVDF in similar ways. In the PM, phase space is divided into cells and the time evolution of the number of electrons in a cell is tracked in a short time step using a transition probability function called propagator (Green's function) which represents the transfer of electrons between cells. Since the change of EVDF is deterministically calculated on the basis of statistical expected values, the PM is characterized by not involving statistical fluctuation unlike MC, and the computational cost is significantly less than that of MC. In particular, for steady-state calculations under a DC electric field, the relaxation-accelerated method¹⁹⁾ achieved convergence about 100 times faster than the conventional method tracking the time evolution of EVDF. Even so, the computational cost was still an issue in the calculation under RF electric fields where the time evolution of EVDF must be tracked. The issue was especially severe at low electric fields, where very fine cell division was necessary. Besides the PM, several studies using equivalent or similar BE-based methods have been made for modeling of RF plasmas and analysis of electron transport under RF electric fields.^{20–27)} However, these methods are not general enough to be used for data preparation for plasma fluid models. The PM is considered to have potential to realize an accurate and practical BE analysis under RF electric fields.

In this work, an improved scheme to calculate the electron advection is presented. In the PM calculation of electron advection across cell boundaries, the conventional upwind difference scheme in the previous code is replaced by a blending scheme where the upwind and the central differences are blended in a certain ratio. This significantly improves the calculation accuracy, the robustness of the PM against coarse meshes, and the computational efficiency of the PM.²⁸⁾ On the basis of the results, a new user-friendly software named BOSPROM has been developed for application to the data supply to fluid models. In this paper, Sect. 2 describes in detail the upwind scheme and the blending scheme used for electron advection calculations. In Sect. 3, we show a benchmark calculation in Ar gas to demonstrate the superiority of the blending scheme over the conventional upwind scheme. Section 4 describes the features of BOSPROM and shows an example calculation under RF electric fields by this software. Section 5 summarizes the present work.

2. Calculation scheme

2.1 Simulation model and governing equation

We consider the time (t) dependent EVDF in velocity (v) space under uniform DC or AC electric field E . The EVDF is denoted as $f(v, \theta, t)$ using polar coordinates (v, θ), where

$v = (v_{\parallel}^2 + v_{\perp}^2)^{1/2}$, $\theta = \arccos(v_{\parallel}/v)$, and $v_{\parallel}$ and $v_{\perp}$ are the velocity components parallel and perpendicular to E , respectively. The EVDF is assumed to be axisymmetric.

The BE under spatially uniform condition is

$$\frac{\partial}{\partial t} f(v, \theta, t) = -\frac{e}{m} E \frac{\partial}{\partial v_{\parallel}} f(v, \theta, t) + \left(\frac{\partial}{\partial t} \right)_{\text{coll}} f(v, \theta, t), \quad (1)$$

where e and m are the electronic charge and mass, respectively. The first and second terms in the right-hand side of Eq. (1) are the acceleration and collision terms, respectively. They represent the change of electron velocity due to the acceleration by E and collisional scattering by background gas molecules.

2.2 Cells configuration

In the PM, velocity space (v, θ) is divided into cells on the basis of the mesh shown in Fig. 1. The PM deals with the number of electrons in each cell, and the intercellular electron transfers due to the electron acceleration and collisional scattering are calculated using acceleration and collision propagators corresponding to the acceleration and collision terms of the BE. Details of the procedure are available in the literature.¹⁹⁾ Practical cells are prepared with a constant $\Delta\varepsilon$, where $\varepsilon = mv^2/2$ is electron energy. This configuration has been adopted to satisfy the energy conservation law in an early PM for spatial development of electron swarms.²⁹⁾ While there is different cell configuration based on constant Δv ,^{30,31)} an advantage of the constant $\Delta\varepsilon$ configuration is that the treatment of the electron energy loss by inelastic collision becomes simple.

The cell is indexed with i and j , which correspond to ε and θ , respectively. Cell (i, j) , denoted as $C_{i,j}$ hereafter, occupies a region of $v_{1\text{eV}}\sqrt{(i-1)\Delta\varepsilon/\varepsilon_{1\text{eV}}} \leq v \leq v_{1\text{eV}}\sqrt{i\Delta\varepsilon/\varepsilon_{1\text{eV}}}$ and $(j-1)\Delta\theta \leq \theta \leq j\Delta\theta$ in velocity space, where $v_{1\text{eV}}$ is the electron speed associated with 1 eV, and $\varepsilon_{1\text{eV}} = 1$ eV. The present cell configuration with constant $\Delta\varepsilon$ results in a coarse resolution around the origin of velocity space, where low-energy electrons are present. This may cause errors in EVDF calculations especially at low DC E or even at intermediate AC E which has low E periods. The present improvement, which will be described later, is to overcome this issue.

2.3 Evaluation of time evolution of EVDF

Starting from some initial distribution, the time evolution of EVDF is tracked for every time step Δt . In this paper, we focus on the electron flow due to the acceleration. (The following formulation is based on the staggered grid generally used in the simulation of fluid flow.) For $C_{i,j}$, number of electrons in the cell is denoted as $n_{i,j}$, and electron density at the cell center is expressed as $\rho_{i,j} = n_{i,j}/V_{i,j}$, where $V_{i,j}$ is the volume of $C_{i,j}$ and $V_{i,j} =$

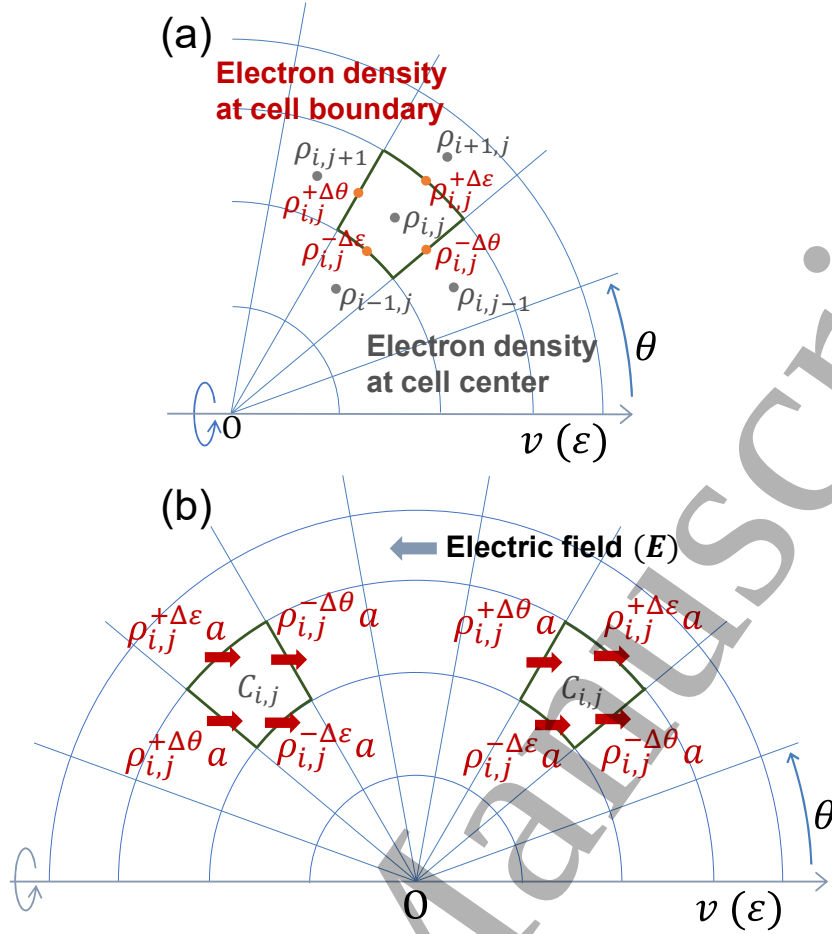


Fig. 1. Calculation cell, definition points of electron density (a), and electron fluxes across the boundary (b).

$\frac{2}{3}\pi\{[\max(v)]^3 - [\min(v)]^3\}\{\cos[\min(\theta)] - \cos[\max(\theta)]\}$ for the v and θ ranges of $C_{i,j}$.¹⁹⁾ The electron densities at cell boundary are defined as in Fig. 1, where location of the boundary is distinguished by superscripts, $+\Delta\epsilon$, $-\Delta\theta$, $-\Delta\epsilon$, and $+\Delta\theta$. Electron flux at the boundary $+\Delta\epsilon$ of $C_{i,j}$ is expressed as $\rho_{i,j}^{+\Delta\epsilon} a$, where a is acceleration ($a = eE/m$). Therefore, the number of electrons flowing across the boundary $+\Delta\epsilon$ during Δt is expressed as $\rho_{i,j}^{+\Delta\epsilon} S_{i,j}^{+\Delta\epsilon} a \Delta t$, where $S_{i,j}^{+\Delta\epsilon}$ is the area of boundary $+\Delta\epsilon$ of $C_{i,j}$ projected to the plane normal to E . $S_{i,j}$ is given as $\pi\{[\max(v_{\perp})]^2 - [\min(v_{\perp})]^2\}$ for the $v_{\perp}$ values on the boundary under consideration.¹⁹⁾ Δt must be short enough to avoid that all electrons in a cell flow out of the cell during Δt . For the other boundaries, electron fluxes are represented as shown in Fig. 1. The number of electrons flowing across each boundary is similarly expressed. When E is oriented leftward as shown in Fig. 1 and $0 \leq \theta < \pi/2$, electrons in $C_{i,j}$ flow out to $C_{i+1,j}$ and $C_{i,j-1}$, whereas electrons in $C_{i-1,j}$ and $C_{i,j+1}$ flow into $C_{i,j}$. The sum of these electrons determines the number of electrons in the cell at the next time step, $n_{i,j}^{\text{new}}$, which can be expressed as follows using the explicit

forward Euler time-integration;

$$\begin{aligned} n_{i,j}^{\text{new}} = & n_{i,j} - a\Delta t \left(\rho_{i,j}^{+\Delta\varepsilon} S_{i,j}^{+\Delta\varepsilon} + \rho_{i,j}^{-\Delta\theta} S_{i,j}^{-\Delta\theta} \right) \\ & + a\Delta t \left(\rho_{i,j}^{-\Delta\varepsilon} S_{i,j}^{-\Delta\varepsilon} + \rho_{i,j}^{+\Delta\theta} S_{i,j}^{+\Delta\theta} \right) + \Delta t \left(\frac{\partial n_{i,j}}{\partial t} \right)_{\text{coll}}, \end{aligned} \quad (2)$$

where the last term is an abbreviated form showing the contribution of collisional scattering by gases.¹⁹⁾ For $\pi/2 \leq \theta < \pi$, electrons in $C_{i,j}$ flow out to $C_{i-1,j}$ and $C_{i,j-1}$, and electrons in $C_{i+1,j}$ and $C_{i,j+1}$ flow into $C_{i,j}$, then

$$\begin{aligned} n_{i,j}^{\text{new}} = & n_{i,j} - a\Delta t \left(\rho_{i,j}^{-\Delta\theta} S_{i,j}^{-\Delta\theta} + \rho_{i,j}^{-\Delta\varepsilon} S_{i,j}^{-\Delta\varepsilon} \right) \\ & + a\Delta t \left(\rho_{i,j}^{+\Delta\varepsilon} S_{i,j}^{+\Delta\varepsilon} + \rho_{i,j}^{+\Delta\theta} S_{i,j}^{+\Delta\theta} \right) + \Delta t \left(\frac{\partial n_{i,j}}{\partial t} \right)_{\text{coll}}. \end{aligned} \quad (3)$$

The time evolution of $n_{i,j}$ is calculated according to the above schemes until $n_{i,j}$ converges to a steady state. The normalized value of EVDF in $C_{i,j}$ is calculated as $(n_{i,j} / \sum_{i,j} n_{i,j}) / V_{i,j}$ at the cell center. For RF E , during a half period in which E orients rightward in Fig. 1, the above calculation scheme should be modified to obtain a mirror image. The calculation is continued until the EVDF reaches a periodic steady state.

2.4 Calculation schemes to evaluate the electron flow

In the previous PM, the electron density at cell boundaries was simply equated with the electron density at the cell-center value on the upstream side; if E is oriented leftward as shown in Fig. 1, the electron densities at cell boundary are expressed as follows:

$$\rho_{i,j}^{+\Delta\varepsilon} = \begin{cases} \rho_{i,j} & \text{for } 0 \leq \theta < \pi/2 \\ \rho_{i+1,j} & \text{for } \pi/2 \leq \theta < \pi \end{cases}, \quad (4)$$

$$\rho_{i,j}^{-\Delta\theta} = \rho_{i,j} \quad \text{for } 0 \leq \theta < \pi, \quad (5)$$

$$\rho_{i,j}^{-\Delta\varepsilon} = \begin{cases} \rho_{i-1,j} & \text{for } 0 \leq \theta < \pi/2 \\ \rho_{i,j} & \text{for } \pi/2 \leq \theta < \pi \end{cases}, \quad (6)$$

$$\rho_{i,j}^{+\Delta\theta} = \rho_{i,j+1} \quad \text{for } 0 \leq \theta < \pi. \quad (7)$$

This is the upwind scheme widely adopted in fluid dynamics, which stabilizes calculations even for the strong advection at high E . The accuracy of this scheme is a first order. However, especially in lower E , the calculation results are very sensitive to $\Delta\varepsilon$. The $\Delta\varepsilon$ value required to obtain sufficient calculation accuracy is very small, which requires a very short Δt to execute a reliable calculation. As a result, the calculation time increases.

Another option for the electron density at cell boundaries is the linearly interpolated

density between adjacent two cells; the electron densities at cell boundary are expressed as

$$\rho_{i,j}^{+\Delta\epsilon} = \frac{V_{i+1,j}\rho_{i,j} + V_{i,j}\rho_{i+1,j}}{V_{i,j} + V_{i+1,j}}, \quad (8)$$

$$\rho_{i,j}^{-\Delta\theta} = \frac{V_{i,j-1}\rho_{i,j} + V_{i,j}\rho_{i,j-1}}{V_{i,j} + V_{i,j-1}}, \quad (9)$$

$$\rho_{i,j}^{-\Delta\epsilon} = \frac{V_{i,j}\rho_{i-1,j} + V_{i-1,j}\rho_{i,j}}{V_{i-1,j} + V_{i,j}}, \quad (10)$$

$$\rho_{i,j}^{+\Delta\theta} = \frac{V_{i,j}\rho_{i,j+1} + V_{i,j+1}\rho_{i,j}}{V_{i,j+1} + V_{i,j}}. \quad (11)$$

This is a central difference scheme weighted by the reciprocal of cell volume. The accuracy of this scheme is a second order. However, in the advective flow, the combination of explicit forward time integration and the central difference (FTCS: Forward Time Centered Space) is known to make the calculation unstable.³²⁾ In the PM, the calculation using the central difference is possible only for diffusive case at very low E .

In order to overcome this situation, we introduce a method to blend the upwind and the central differences in a ratio ξ ($0 \leq \xi \leq 1$), where ξ is called the blending factor. Here, $\xi = 0$ corresponds to the pure upwind and $\xi = 1$ is the pure central difference. This method is expected to have intermediate characteristics of both the upwind and the central differences. Basic idea of this method was proposed for the fluid flow calculation, where the method was originally called hybrid scheme.^{33,34)} Nowadays, this blending scheme is built in most fluid dynamics software packages, e.g., OpenFOAM³⁵⁾ and ANSYS Fluent.³⁶⁾ Although situations are quite different, the widely used Scharfetter–Gummel scheme^{37,38)} in plasma fluid modelings is similar to this blending method; in the Scharfetter–Gummel scheme, the difference scheme is smoothly connected from the central difference to the upwind difference via the Peclet number (the ratio of advection flux to diffusion flux). In the present blending method, the electron densities at cell boundary are expressed as follows:

$$\rho_{i,j}^{+\Delta\epsilon} = \begin{cases} \frac{V_{i+1,j}\rho_{i,j} + \xi V_{i,j}\rho_{i+1,j}}{\xi V_{i,j} + V_{i+1,j}} & \text{for } 0 \leq \theta < \pi/2 \\ \frac{\xi V_{i+1,j}\rho_{i,j} + V_{i,j}\rho_{i+1,j}}{V_{i,j} + \xi V_{i+1,j}} & \text{for } \pi/2 \leq \theta < \pi \end{cases}, \quad (12)$$

$$\rho_{i,j}^{-\Delta\theta} = \frac{V_{i,j-1}\rho_{i,j} + \xi V_{i,j}\rho_{i,j-1}}{\xi V_{i,j} + V_{i,j-1}} \quad \text{for } 0 \leq \theta < \pi, \quad (13)$$

$$\rho_{i,j}^{-\Delta\epsilon} = \begin{cases} \frac{V_{i,j}\rho_{i-1,j} + \xi V_{i-1,j}\rho_{i,j}}{\xi V_{i-1,j} + V_{i,j}} & \text{for } 0 \leq \theta < \pi/2 \\ \frac{\xi V_{i,j}\rho_{i-1,j} + V_{i,j-1}\rho_{i,j}}{V_{i,j-1} + \xi V_{i,j}} & \text{for } \pi/2 \leq \theta < \pi \end{cases}, \quad (14)$$

$$\rho_{i,j}^{+\Delta\theta} = \frac{V_{i,j}\rho_{i,j+1} + \xi V_{i,j+1}\rho_{i,j}}{\xi V_{i,j+1} + V_{i,j}} \quad \text{for } 0 \leq \theta < \pi. \quad (15)$$

It is a problem how to determine ξ . In the calculation of fluid flow, the Peclet number was utilized to estimate the ξ value.³⁴⁾ In the PM, however, it is difficult to adopt such a method, because the diffusion processes are calculated on the basis of collisional scattering probabilities, therefore a convenient parameter such as the Peclet number cannot be defined. In this work, a trial-and-error approach is employed to determine the ξ value; we set $\xi = 1$ at the beginning of the calculation. If advection is strong for given $\Delta\varepsilon$ or Δt , $n_{i,j}^{\text{new}}$ in Eq. (2) or (3) may become negative and the calculation might fail. In this case, the calculation is redone from the beginning after subtracting a small value (typically 0.02) from ξ . In the actual calculation, if initial EVDF is far from the final distribution in periodic steady state, the ξ value quickly decreases during the iterative calculation. This means that the calculation accuracy is also reduced. In order to avoid this, the calculation is sometimes performed in two steps. First, an approximate EVDF is calculated with rough mesh. Next, the calculation with fine mesh is made with resetting ξ as $\xi = 1$ and using the approximate EVDF as an initial condition. This is effective to preserve the accuracy when only the final EVDF in periodic steady state is concerned, such as in applications to plasma fluid modeling.

3. Verification

3.1 Electron energy distribution function

For a benchmark of the blending method, PM calculations for the EVDF in Ar have been carried out under the following conditions; gas pressure p is 133 Pa, temperature is 273 K, the frequency f of RF electric field $E \propto \cos(2\pi ft)$ is 13.56 MHz, its rms magnitude as reduced electric field E_{rms}/N is 0.33 Td (N is gas molecule number density, and 1 Td = 10^{-21} Vm²). The presence of metastable excited species Ar* is considered in this benchmark and the mole ratio is assumed to be Ar : Ar* = 0.9999 : 0.0001. Maximum energy ε_{max} for the EVDF calculation is 6.0 eV, and Δt is 12.8 ps. The ε_{max} value is determined so that the ratio, the value of electron energy probability function (EPPF) at $\varepsilon = \varepsilon_{\text{max}}$ to the maximum value of EPPF, is less than a small value, e.g. 10^{-6} . Here, EPPF is defined as $F(\varepsilon)/\sqrt{\varepsilon}$ and $F(\varepsilon)$ is the electron energy distribution function (EEDF). This criterion for ε_{max} ensures the swarm parameters, which are obtained by energy integral calculation from 0 to ε_{max} , are sufficiently accurate for practical use in plasma fluid models. The value of Δt is determined empirically so that the calculation results are reasonable avoiding that all electrons in a cell flow out during Δt .¹⁹⁾ The resolution of θ is fixed at $\Delta\theta = \pi/90$. The cross section data have been taken from the literature³⁹⁾ and the TRINITI database of LXCat.^{40,41)} The collisional processes include elastic

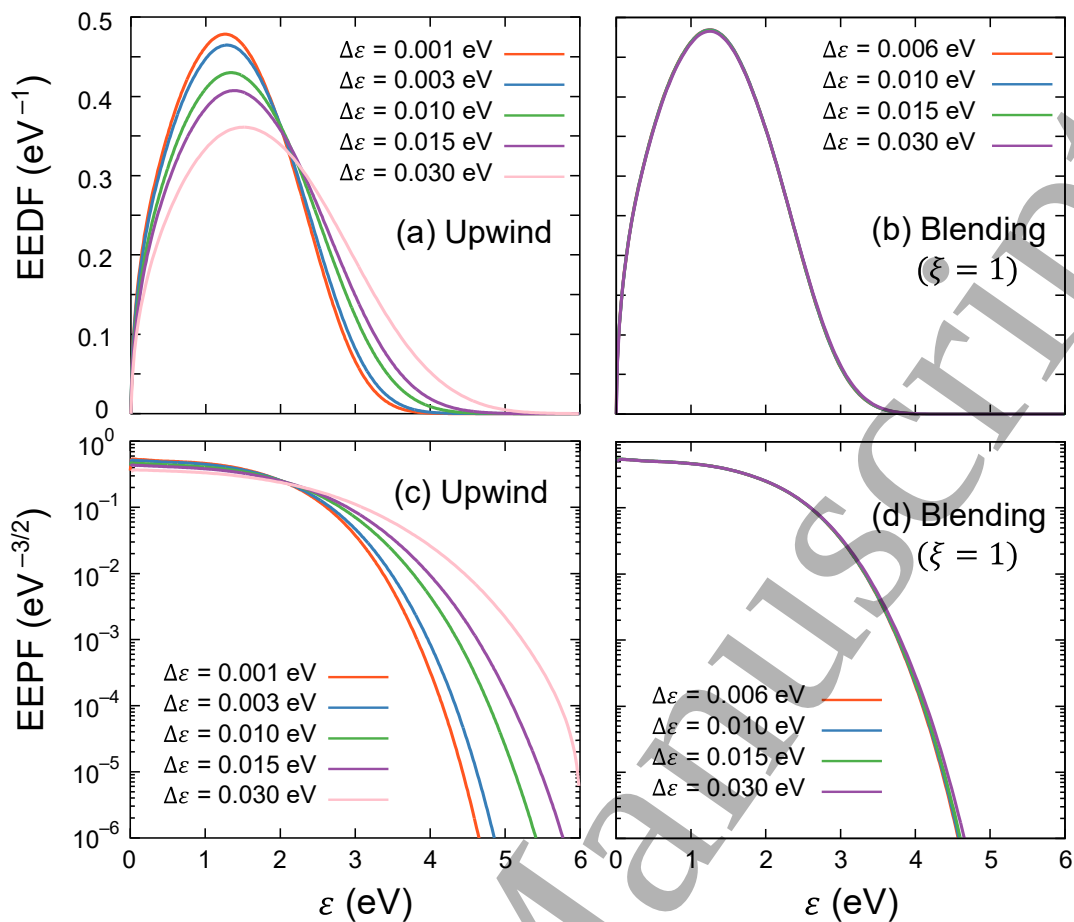


Fig. 2. EEDFs and EEPFs calculated by the upwind scheme, (a) and (c), and the blending scheme, (b) and (d), at $E_{\text{rms}}/N = 0.33$ Td.

collision, excitations (thresholds, 11.55 and 12.90 eV), ionization (15.76 eV), and stepwise ionization of Ar^* (4.20 eV). The energy loss at the elastic collisions is considered with the mass ratio m/M between an electron and an Ar atom. Usually, this energy loss becomes smaller than the energy resolution $\Delta\epsilon$. In the calculation of elastic collision propagator, we can employ the method that the number of electrons transferred to the energy ϵ_d , where $\epsilon_i \leq \epsilon_d < \epsilon_{i+1}$ (ϵ_i and ϵ_{i+1} are the cell-center values of energy), is distributed to the two cells, $C_{i,j}$ and $C_{i+1,j}$, with weighting factors, w_i and $1 - w_i$, respectively; w_i is determined from $\epsilon_d = w_i\epsilon_i + (1 - w_i)\epsilon_{i+1}$. This method has been also employed in the calculation of excitation- and ionization-collision propagators.¹⁹⁾ EEDFs and EEPFs calculated for several different $\Delta\epsilon$ values by the upwind and the blending schemes are compared as shown in Fig. 2.

Under RF E , EVDF and related swarm parameters oscillate with time. The EEDF and the EEPF shown in Fig. 2 are those at the phase that E takes its maximum. Because E_{rms}/N is small, the values of oscillation amplitude of EEDF and EEPF are small as well; the differences

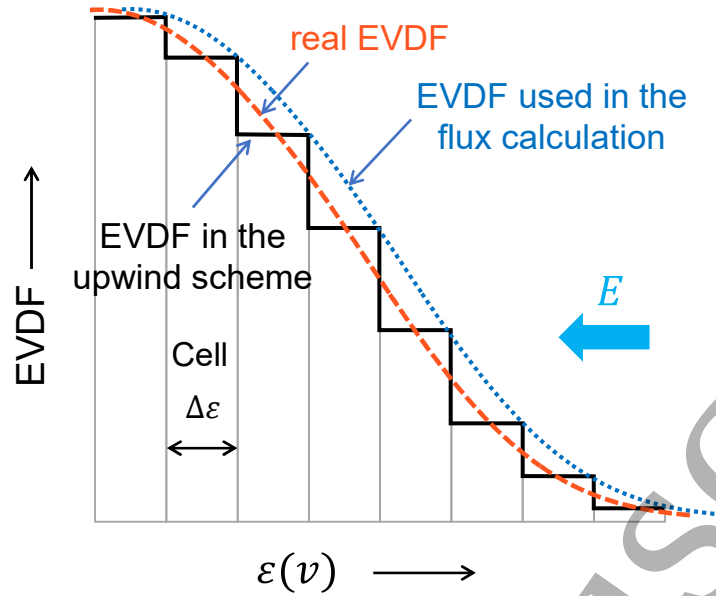


Fig. 3. Schematic illustration of EVDF in the upwind scheme (solid stepwise curve), real EVDF (broken curve), and EVDF used in the flux calculation by the upwind scheme (dotted curve).

by the phase are not observable in the figure. In the upwind case, the shapes of EEDF and EEPF change greatly depending on $\Delta\epsilon$, and the peak of the EEDF shifts to the higher-energy side as $\Delta\epsilon$ increases. On the other hand, in the blending case, such a tendency is too small to recognize on the graph scale of Fig. 2(b). The logarithmic plot of EEPFs by the blending scheme in Fig. 2(d) clearly shows that the EEPF curves agree well with each other up to the high- ϵ tail regardless of $\Delta\epsilon$, which indicates that the blending scheme works effectively. In this case, FTCS ($\xi = 1$) calculation is possible owing to the very small value of E_{rms}/N .

In the PM calculation by the upwind scheme, EVDF can be regarded as a stepwise curve as schematically shown in Fig. 3, because cell-center values of electron density are used in the electron flux evaluation at the cell boundaries. In the electron flux calculation, this is equivalent to use a virtual EVDF shifted by a half of $\Delta\epsilon$ to the higher-energy side as shown by a dotted curve in Fig. 3. This causes an overestimation of the electron flux at cell boundaries. Larger $\Delta\epsilon$ makes the overestimation more serious. It can be considered that the increase of $\Delta\epsilon$ is equivalent to the increase of effective E , which results in the EEDF shape variation with $\Delta\epsilon$ in Figs. 2(a) and 2(c). This demerit of the upwind scheme is significantly reduced in the blending scheme as shown in Figs. 2(b) and 2(d).

3.2 Mean energy, drift velocity, and ionization frequency

Time evolution of mean electron energy $\langle\epsilon\rangle$, drift velocity W , and total ionization frequency ν_{ion} can be calculated from $\langle\epsilon\rangle = \left(\sum_{i,j} \epsilon_i n_{i,j}\right) / \left(\sum_{i,j} n_{i,j}\right)$, $W =$

$\left(\sum_{i,j} v_i \cos \theta_j n_{i,j} \right) / \left(\sum_{i,j} n_{i,j} \right)$, and $v_{\text{ion}} = \left(\sum_k \sum_{i,j} N_k \sigma_{i,k} v_i n_{i,j} \right) / \left(\sum_{i,j} n_{i,j} \right)$ using the cell-center values of ε_i , v_i , θ_j , and $n_{i,j}$, where N_k and $\sigma_{i,k}$ are number density and ionization cross section of the k th species, respectively (the calculation procedure for each parameter is the same in both the upwind and the blending schemes). Figures 4(a)–4(c) show the $\Delta\varepsilon$ dependence of rms of $\langle\varepsilon\rangle$, $\langle\varepsilon\rangle_{\text{rms}}$, rms of W , W_{rms} , and rms of reduced total ionization frequency, $v_{\text{ion,rms}}/N$, calculated at several E_{rms}/N values by the upwind and the blending schemes; in Fig.4(c), results at $E_{\text{rms}}/N = 0.33$ Td are excluded because their values are too small to discuss the precision of the schemes. In these calculations, how ξ varies depending on $\Delta\varepsilon$ is also shown in Fig. 4(d). Calculation conditions at $E_{\text{rms}}/N = 0.33, 1.0, 10$, and 50 Td were $\varepsilon_{\text{max}} = 6.0, 13.2, 22.0$, and 24.1 eV and $\Delta t = 12.8, 6.4\text{--}51.2, 1.6\text{--}12.8$, and $0.4\text{--}3.2$ ps (depending on $\Delta\varepsilon$), respectively. The other conditions on the gas and the PM were unchanged from those set in the preceding subsection.

In the upwind case, $\langle\varepsilon\rangle_{\text{rms}}$ and $v_{\text{ion,rms}}/N$ remarkably increase, and W_{rms} decreases with the increase of $\Delta\varepsilon$, especially at lower E . On the other hand, in the blending case, $\langle\varepsilon\rangle_{\text{rms}}$, W_{rms} , and $v_{\text{ion,rms}}/N$ are almost insensitive to $\Delta\varepsilon$ in the examined ranges of $\Delta\varepsilon$. Although the values of $v_{\text{ion,rms}}/N$ are very small, because the verifications are made mainly at lower E_{rms}/N , the advantage of the blending scheme is clear. At higher E , the differences of these parameters between the upwind and the blending schemes become small. On average, ξ tends to decrease as E_{rms}/N increases. The small ξ value is caused by the strong advection at high E ; the stable calculation is possible only with small ξ , where the calculation scheme are close to the upwind one. The value of ξ also decreases as $\Delta\varepsilon$ decreases at a constant $E_{\text{rms}}/N \geq 1$ Td. Especially, at $E_{\text{rms}}/N = 50$ Td, the amount of the variation of ξ with $\Delta\varepsilon$ is about 0.7. However, at the high E_{rms}/N values, the effect of $\Delta\varepsilon$ on the swarm parameters is basically small; the large variation of ξ is not a problem for practical use.

3.3 Calculation speed

Computational efficiency of the upwind and the blending schemes was roughly evaluated and compared using a CPU of Intel Core i7-6700 (3.4 GHz) and execution programs build by GNU GCC g++ compiler of MinGW-w64⁴²⁾ on Microsoft Windows 10 system. Elapsed times of calculation by both schemes at $E_{\text{rms}}/N = 0.33$ and 10 Td are plotted as a function of $\Delta\varepsilon$ in Fig. 5, where the elapsed time by the blending scheme contains the time for the trial-and-error process to determine ξ . The calculation conditions were the same as those in Fig. 4.

As we are interested in not only calculation speed but also accuracy of the scheme, the error of $\langle\varepsilon\rangle_{\text{rms}}$, $\delta_{\langle\varepsilon\rangle}$, is estimated using a $\langle\varepsilon\rangle_{\text{rms}}$ value extrapolated by $\Delta\varepsilon \rightarrow 0$ in Fig. 4. In

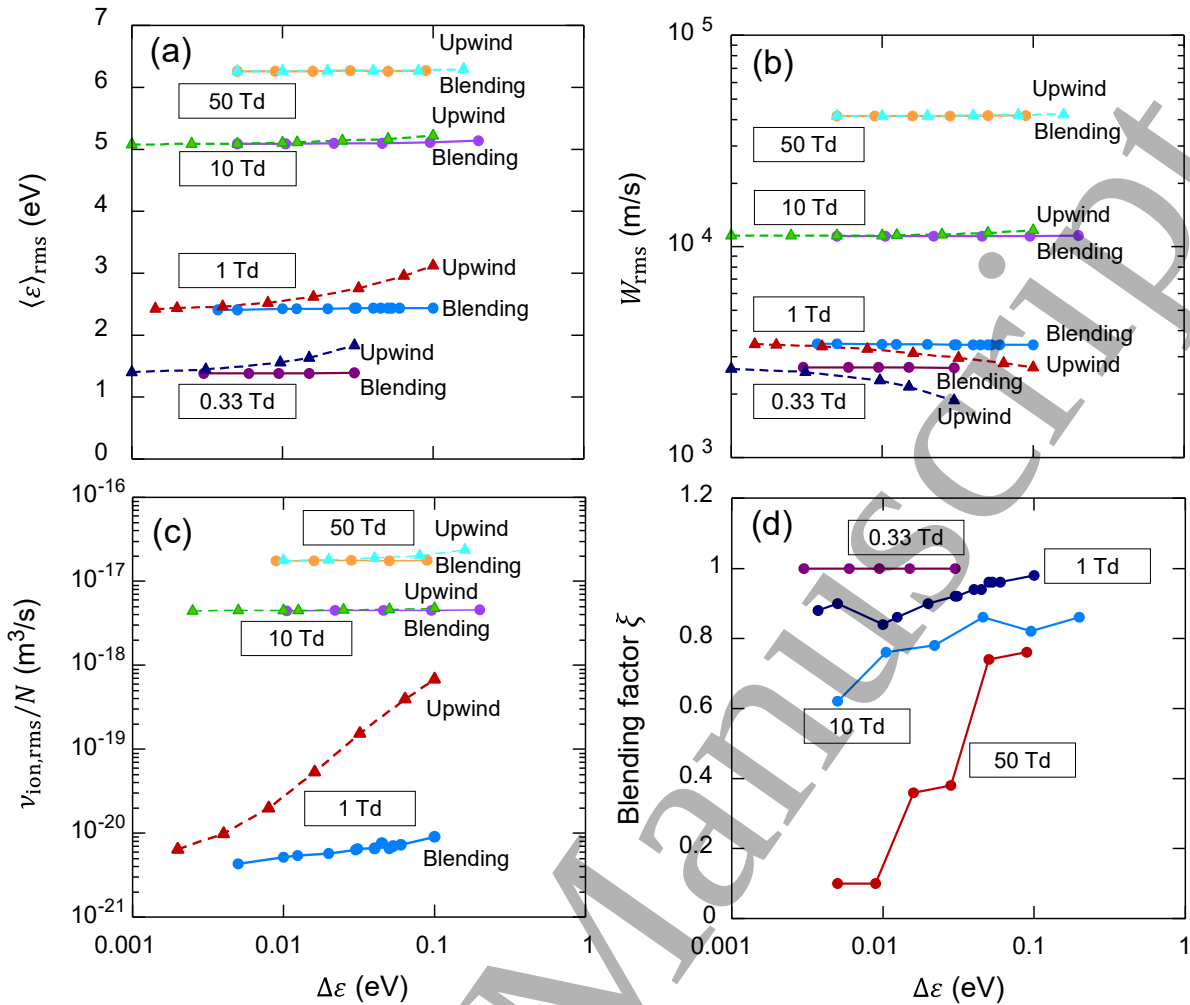


Fig. 4. Time averaged mean electron energy $\langle\epsilon\rangle_{\text{rms}}$ (a), time averaged drift velocity W_{rms} (b), time averaged reduced ionization frequency $\nu_{\text{ion,rms}}/N$ (c), and blending factor ξ (d) as functions of $\Delta\epsilon$ for $E_{\text{rms}}/N = 0.33$, 1.0, 10, and 50 Td.

Fig. 5, circle area represents the magnitude of $\delta_{\langle\epsilon\rangle}$ (the accompanying number is its value in percent). Of course, the blending scheme increases complexity of the PM calculation and the elapsed time compared to the upwind scheme at the same $\Delta\epsilon$. However, considering the acceptable $\delta_{\langle\epsilon\rangle}$, a larger value of $\Delta\epsilon$ is allowed in the blending scheme. This improves the overall efficiency of PM calculation procedure, and can significantly reduce the total computation time. This feature is more significant at lower E . The blending scheme can speed up the calculation by more than one order of magnitude at $E_{\text{rms}}/N = 0.33$ Td. In contrast, at $E_{\text{rms}}/N = 10$ Td, the efficiency gain of the blending scheme is relatively small, which can be recognized by the difference of $\delta_{\langle\epsilon\rangle}$ (difference of circle areas in Fig. 5) between the upwind and the blending schemes; the differences at $E_{\text{rms}}/N = 10$ Td are smaller than those

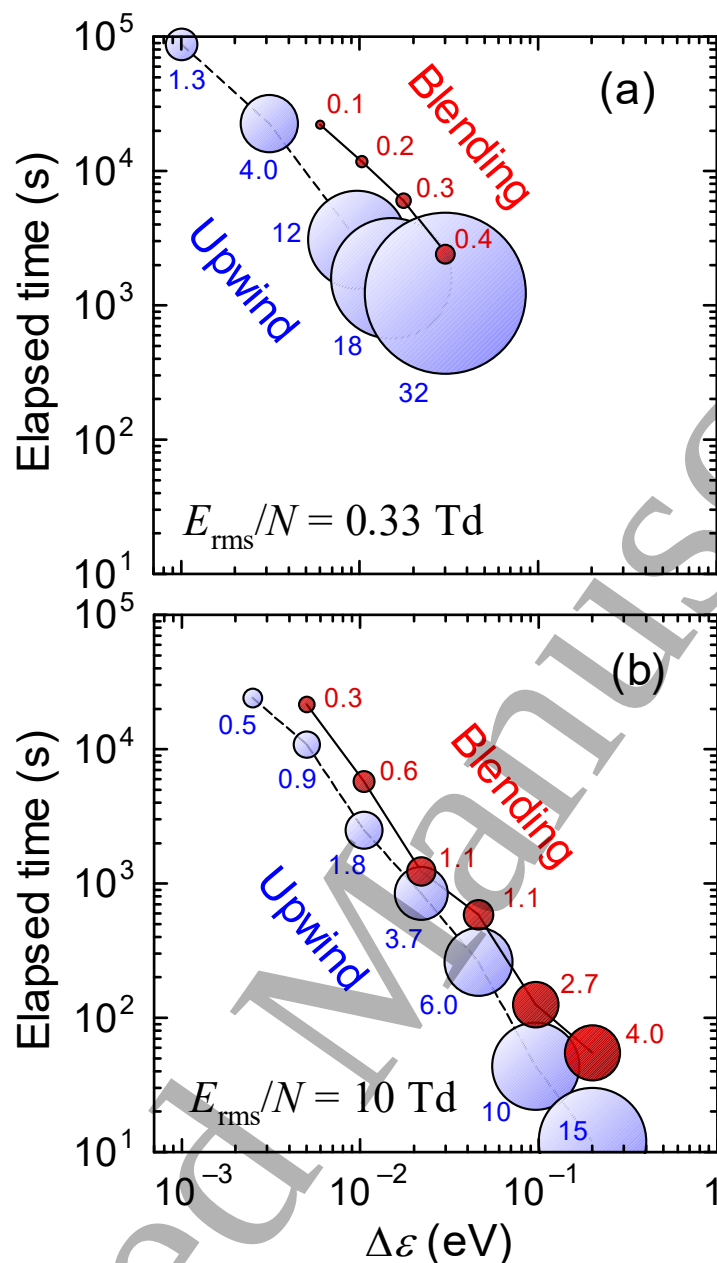


Fig. 5. Computational elapsed time of the upwind and blending schemes as a function of $\Delta\epsilon$ at $E_{\text{rms}}/N = 0.33 \text{ Td}$ (a) and 10 Td (b). Circle area and accompanying number represent $\delta_{\langle\epsilon\rangle}$, which is estimated error of $\langle\epsilon\rangle_{\text{rms}}$ in percent (not the error range of the elapsed time).

at $E_{\text{rms}}/N = 0.33 \text{ Td}$. This is equivalent to the tendency shown in Fig. 4.

3.4 Reduced electric field dependence of swarm parameters

The data of $\langle\epsilon\rangle_{\text{rms}}$, W_{rms} , and $v_{\text{ion,rms}}/N$ were calculated for a series of E_{rms}/N values by the upwind and the blending schemes. Results are shown and compared in Figs. 6(a)–6(c). The $\Delta\epsilon$ values used in the calculation are shown in Fig. 6(d), and the resulting ξ value is shown in

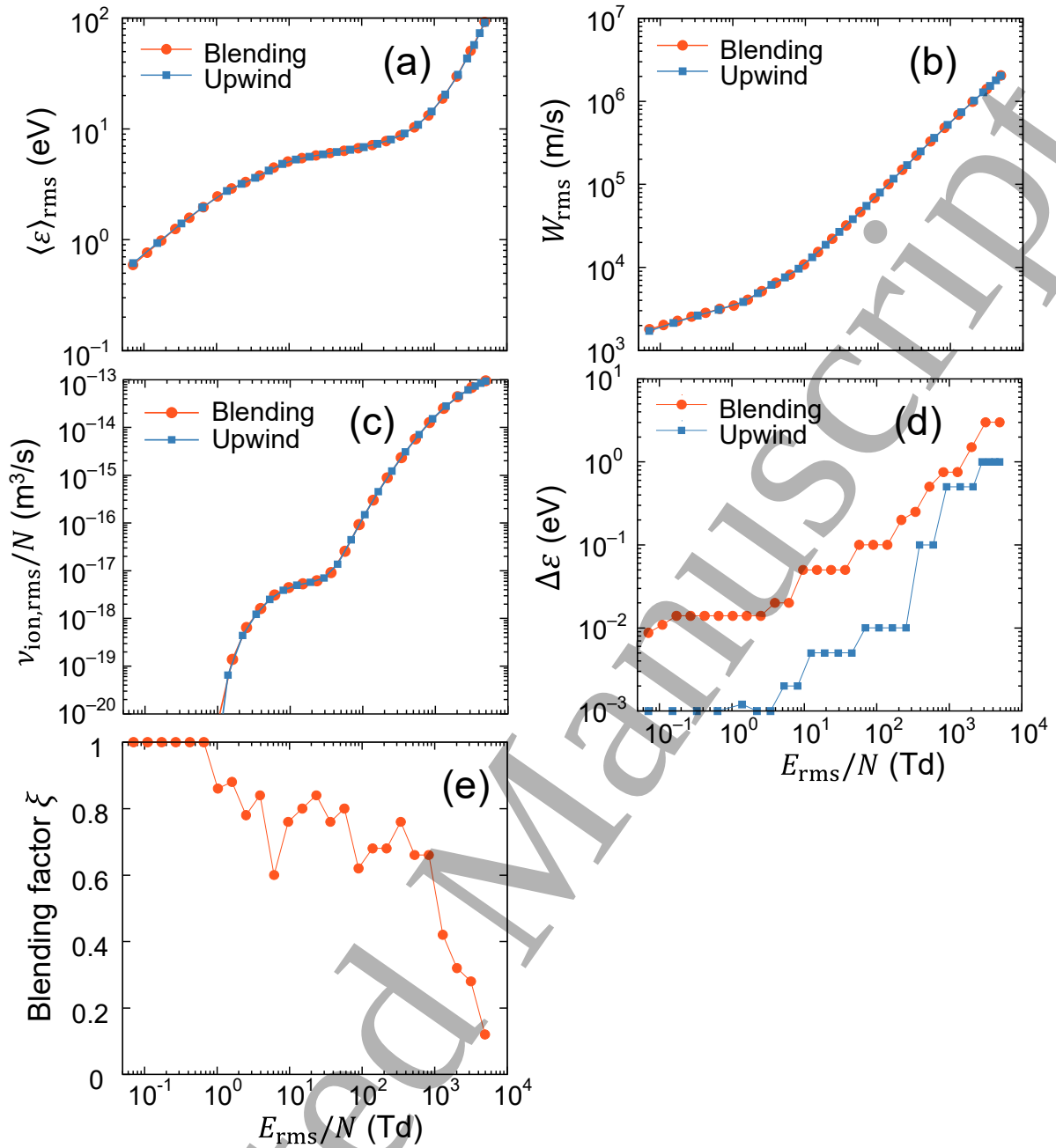


Fig. 6. The E_{rms}/N dependences of $\langle \epsilon \rangle_{\text{rms}}$ (a), W_{rms} (b), and $\nu_{\text{ion,rms}}/N$ (c) calculated by the upwind and the blending schemes under the conditions of $\Delta \epsilon$ (d) and ξ (e). A shoulder of $\nu_{\text{ion,rms}}/N$ in the region of $E_{\text{rms}}/N \lesssim 30$ Td is due to the ionization of Ar^* .

Fig. 6(e). In the upwind case, we used a sufficiently fine value of $\Delta \epsilon$ for each value of E_{rms}/N . Although considerably large $\Delta \epsilon$ value was used in the blending case, results by the upwind and the blending schemes agreed well with each other. Especially, it is notable that $\Delta \epsilon$ values 10 times larger than those of the upwind case are acceptable at lower E .

These results show that the blending scheme is robust against the coarse mesh, which is

practically very useful to reduce the computation time. Although the ξ values shown in Fig. 6(e) are kept to be 1.0 at lower E_{rms}/N , its values are somewhat fluctuated at $E_{\text{rms}}/N \gtrsim 1$ Td. This may be due to the trial-and-error process to determine ξ . However, this level of fluctuation is too small to affect the swarm parameters.

4. Computer software

4.1 Features of the software

On the basis of the results mentioned above, we have developed a new user-friendly computer program named BOSPROM (Boltzmann Solver by Propagator Method),⁴³⁾ which is an application on the Microsoft Windows system. Characteristic features of the program are listed as follows:

- (1) A user-friendly graphical-user-interface is equipped;
- (2) The data of the LXCat database^{40,41)} can be directly read and handled;
- (3) Parallel computation by multi-processes for a series of E values is possible;
- (4) Lookup tables applicable to plasma fluid models can be easily created by parallel computing;
- (5) Fast calculation with rough mesh is available, which is useful for quickly making electron-temperature-based lookup tables;
- (6) For DC E , the relaxation-accelerated method¹⁹⁾ is employed, which drastically speeds up the computation;
- (7) For RF E , the blending method introduced by this paper is employed, which makes the practical calculation for RF E possible; and
- (8) Exact calculations under extreme conditions, such as at very strong E or in strongly electronegative gases, are possible, where the calculation by the two-term approximation sometimes fails.

Among these features, the most beneficial and advanced one is (7); the software realizes a practical BE analysis under RF E . Previously, this type of analysis was reported to be also possible by a two-term approximation software such as BOLSIG+.¹¹⁾ However, in BOLSIG+, the frequency of E should be much higher than the collision frequency, which restricts the applicable frequency to a gigahertz range (microwave discharges). Although several other methods of BE-related analysis under RF E have been known,^{20–27)} BOSPROM is regarded as the first general use software which enables a practical and exact RF analysis of BE.

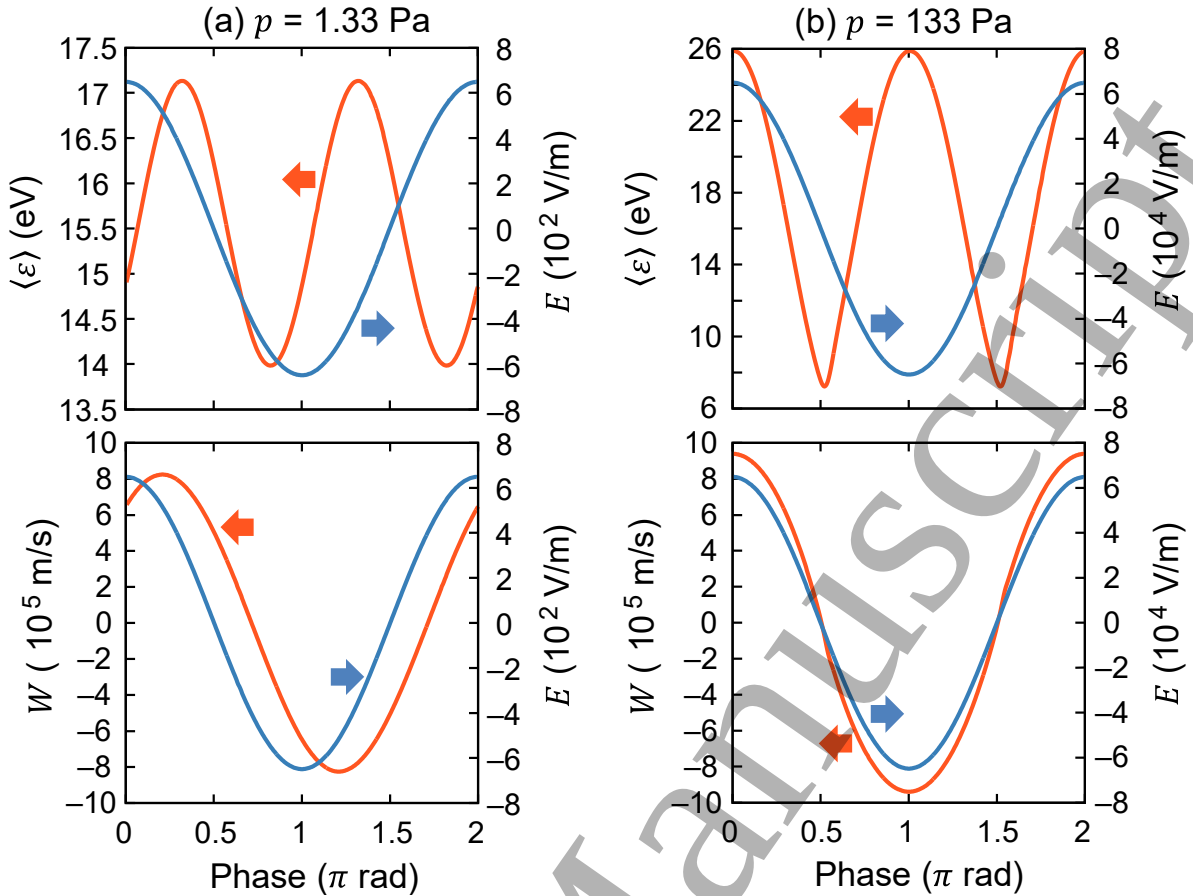


Fig. 7. Time evolutions of $\langle \varepsilon \rangle$ and W under the sinusoidal RF electric field of $E_{\text{rms}}/N = 1298$ Td at $p = 1.33$ (a) and 133 Pa (b).

4.2 Phase shift in mean energy and drift velocity under RF E

As another example for feature (7), responses of $\langle \varepsilon \rangle$ and W to the sinusoidal RF E are shown in Fig. 7, where time evolutions of $\langle \varepsilon \rangle$ and W during one period in the periodic steady state is plotted with the RF E (shown on the right axis) of $E_{\text{rms}}/N = 1298$ Td at the gas pressures p of 1.33 and 133 Pa. Calculation conditions at $p = 1.33$ and 133 Pa were $\varepsilon_{\text{max}} = 800$ and 300 eV, $\Delta\varepsilon = 0.25$ and 0.89 eV, $\Delta t = 12.8$ and 0.2 ps, and typical $\xi = 0.04$ and 0.1 , respectively. Other conditions were the same as those in Sect. 3. Both $\langle \varepsilon \rangle$ and W oscillate with E , where the oscillation frequency of $\langle \varepsilon \rangle$ is $2f$. Remarkable phase delays are recognized in the wave forms of $\langle \varepsilon \rangle$ and W at $p = 1.33$ Pa. This means that electrons cannot fully follow the time variation of the RF E , which is one of the well-known characteristics of RF nonequilibrium plasmas. The phase delays in $\langle \varepsilon \rangle$ and W (denoted as $\Delta\phi_{\langle \varepsilon \rangle}$ and $\Delta\phi_W$) are obtained from the phase at the maximum peak in the wave forms; their values are $\Delta\phi_{\langle \varepsilon \rangle} = 0.32\pi$ and $\Delta\phi_W = 0.21\pi$. With increasing p , the phase delay becomes small. At $p = 133$ Pa, the phase delays almost

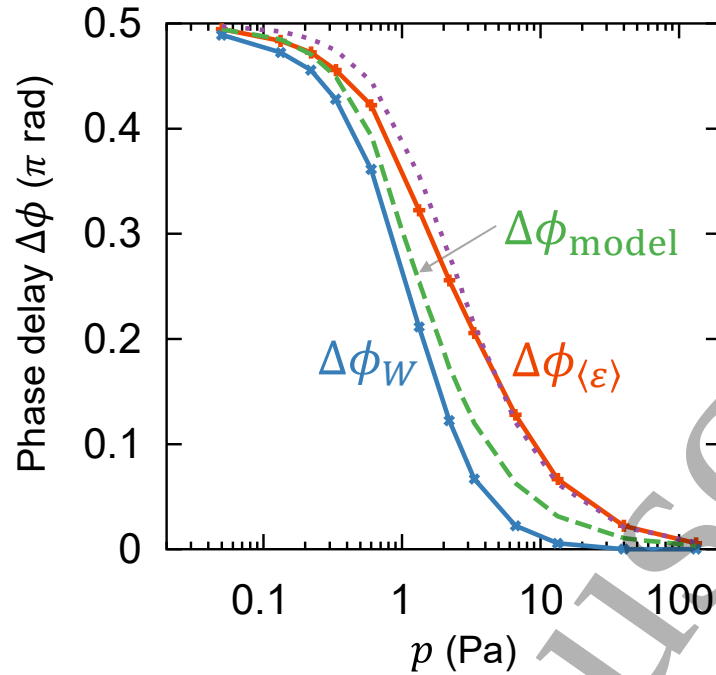


Fig. 8. Phase delays in $\langle \varepsilon \rangle$ and W ($\Delta\phi_{\langle \varepsilon \rangle}$ and $\Delta\phi_W$) at $E_{\text{rms}}/N = 1298 \text{ Td}$ as functions of p . $\Delta\phi_{\text{model}}$ is the phase delay of electron velocity in the constant-collision-frequency model, $\arctan(2\pi f/\nu_{\text{total}})$. Dotted curve is $\arctan(4\pi f/\nu_{\text{total}})$.

disappear leaving only about $5.6 \times 10^{-3}\pi$ in $\langle \varepsilon \rangle$ (this is the resolution of data); the value obtained from the phase at which $\langle \varepsilon \rangle$ takes the minimum in the wave form is about 0.022π . It should be noted that the wave form of $\langle \varepsilon \rangle$ is deformed from a simple sinusoidal one. With increasing p , the values of $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} also increase; the oscillation amplitudes of $\langle \varepsilon \rangle$ and W increase as well.

The data of $\Delta\phi_{\langle \varepsilon \rangle}$ and $\Delta\phi_W$ are calculated for several different p values and shown in Fig. 8 as functions of p . As a general trend, with decreasing p , $\Delta\phi_{\langle \varepsilon \rangle}$ and $\Delta\phi_W$ increase and approach to $\pi/2$. Throughout in the examined p range, $\Delta\phi_{\langle \varepsilon \rangle} > \Delta\phi_W$. This is reasonable behavior, since the energy relaxation time τ_e is known to be longer than the momentum relaxation time τ_m .^{38,44)} Incidentally, the relationship $\tau_e > \tau_m$ is confirmed as follows. Representations of τ_m and τ_e are given as $\tau_m = mW/eE$ (under DC E) and $\tau_e = [(2m/M)\nu_{\text{elastic}} + (\sum_k \varepsilon_{\text{ex},k} \nu_{\text{ex},k})/\langle \varepsilon \rangle + (\sum_k \varepsilon_{\text{ion},k} \nu_{\text{ion},k})/\langle \varepsilon \rangle]^{-1}$.⁴⁴⁾ Here, ν_{elastic} is the frequency of elastic collision, and $\nu_{\text{ex},k}$ and $\nu_{\text{ion},k}$ are those of excitation and ionization (thresholds: $\varepsilon_{\text{ex},k}$ and $\varepsilon_{\text{ion},k}$) for the k th excited and ionic species, respectively. In the present case at $p = 1.33 \text{ Pa}$, the estimated value of $\tau_e = 105 \text{ ns}$ is much longer than that of $\tau_m = 8.8 \text{ ns}$ for the reduced DC electric field of 1298 Td . Both relaxation times are inversely proportional to p as expected from the above formulae.

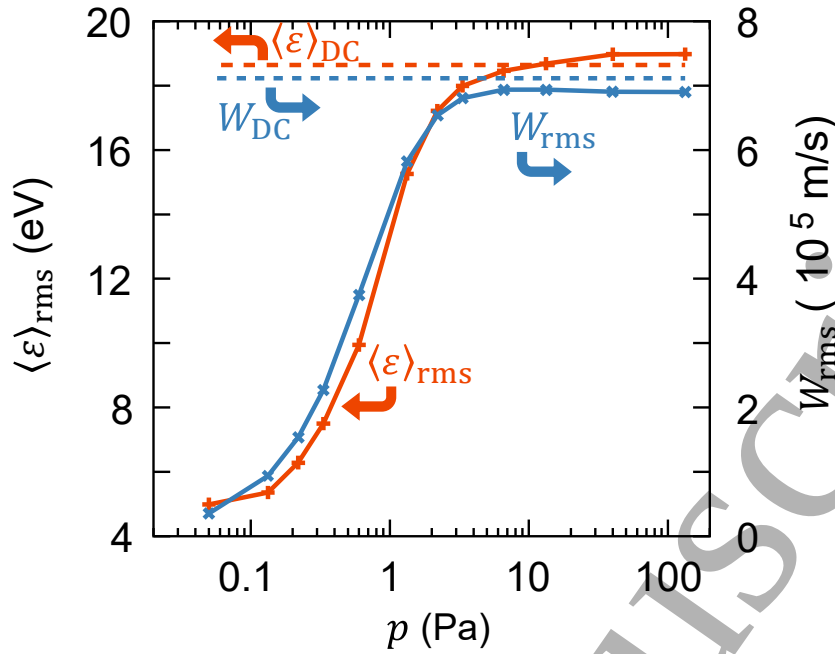


Fig. 9. $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} at $E_{\text{rms}}/N = 1298 \text{ Td}$ as functions of p . Broken lines show $\langle \varepsilon \rangle_{\text{DC}}$ and W_{DC} for DC electric field of $E/N = 1298 \text{ Td}$.

In a simple constant-collision-frequency model, the phase delay of the electron velocity is given as $\arctan(2\pi f/\nu_{\text{total}})^{45,46}$ (ν_{total} is total collision frequency), from which the phase delay can be estimated. Using the rms value of ν_{total} , the phase delay of electron velocity, $\Delta\phi_{\text{model}}$, is estimated and also shown in Fig. 8 with broken line. Overall, $\Delta\phi_W$ obtained by the PM calculation coincides with $\Delta\phi_{\text{model}}$, though the model is rather simple. The calculated result of $\Delta\phi_W$ shown in Fig. 8 is considered to be reasonable. It seems that calculated $\Delta\phi_{\langle \varepsilon \rangle}$ is well approximated as $\arctan(4\pi f/\nu_{\text{total}})$, which is shown in Fig. 8 with the dotted curve. Although it is unclear whether this formula has any physical background, this may be useful for some cases as an empirical approximation.

The dependence of $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} on p obtained from the above calculations are shown in Fig. 9. At higher p , $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} are almost constant, while they decrease with decreasing p below around 10 Pa, at which the phase delays in $\langle \varepsilon \rangle$ and W also start to increase with decreasing p as shown in Fig. 8. These results reflect that electrons cannot fully follow the RF E and it is difficult for them to obtain the energy from E , which is considered to be typical characteristics of RF nonequilibrium plasmas at low p . This corresponds to the behavior that the EVDF is still in the process of relaxing to the so-called drift equilibrium where the relaxation of EVDF is completed. Figures 8 and 9 represent the transition from equilibrium to nonequilibrium in the electron drift under RF E with decreasing p .

In Fig. 9, the mean electron energy $\langle \varepsilon \rangle_{\text{DC}}$ and the drift velocity W_{DC} for DC electric field of $E/N = 1298 \text{ Td}$ are also shown with broken lines and compared to $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} . Although the physical background of this comparison is ambiguous, such a comparison is interesting from a practical viewpoint of parameter adjustment in plasma fluid models. $\langle \varepsilon \rangle_{\text{DC}}$ and W_{DC} are independent of p since E/N is assumed to be constant. At higher p , though the values of $\langle \varepsilon \rangle_{\text{DC}}$ and W_{DC} are close to those of $\langle \varepsilon \rangle_{\text{rms}}$ and W_{rms} , respectively, there exists some amount of difference between the values of DC and RF cases; there are relations $\langle \varepsilon \rangle_{\text{DC}} < \langle \varepsilon \rangle_{\text{rms}}$ and $W_{\text{DC}} > W_{\text{rms}}$. As p decreases, the relations become $\langle \varepsilon \rangle_{\text{DC}} > \langle \varepsilon \rangle_{\text{rms}}$ and $W_{\text{DC}} > W_{\text{rms}}$. The discrepancy between the values of DC and RF cases become large with decreasing p . However, it is not clear how the difference in the parameters between DC and RF cases affects the results of plasma fluid models.

As shown in Figs. 7–9, BOSPROM can provide the important information about the electron kinetics under RF E , which is expected to contribute to the understanding of RF nonequilibrium plasmas.

4.3 Future issues

Unfortunately, for the application of swarm parameters to plasma fluid models, the advanced feature of BOSPROM cannot be fully utilized, because the most commonly used plasma fluid models do not properly reflect nonequilibrium features of the RF plasmas such as phase delay of the swarm parameters. At present, only swarm parameters ignoring the phase information may be used for general plasma fluid models, but there is no physical justification in such a treatment. Nevertheless, in some preliminary studies by a general plasma fluid model, we have experienced that the swarm parameters obtained by ignoring the phase information under RF E yielded slightly better simulation results than those obtained under DC E . It is expected that more advanced models such as the relaxation-continuum model^{38,47,48)} will be commonly used to achieve practical simulations of RF nonequilibrium plasmas.

The most attractive characteristics of the conventional two-term approximation is the low computational cost; typical elapsed time of calculation by BOLSIG+ is less than a few seconds, whereas it is tens of minutes for BOSPROM at low E_{rms}/N . It is efficient to choose the appropriate method depending on the situation and purpose. However, it is not yet fully understood which method should be selected to calculate swarm parameters depending on given circumstances and how the simulation results of plasma fluid models differ depending on the selected method. These are important issues to be addressed in future.

Another demand would be the consideration of Coulomb collisions, which is important

in high-density plasmas. Since its calculation algorithm by two-term approximation has been established,^{11,49)} its implementation is expected also in the PM.

5. Conclusions

In the calculation of electron flow in the PM for solving the BE, we focused on the method how to evaluate the electron flux across cell boundaries due to the acceleration by E , and reconsidered the calculation schemes. The upwind scheme used in the previous PM was stable even for strong advection at high E , but very fine cells were required to obtain sufficiently accurate results at low E , which made the computational cost high. Though the central difference is an ideal scheme, this was unstable for the advection flow. A new improved scheme for the electron flow calculation across cell boundaries was proposed in the present work, where the upwind and central difference schemes were blended in a ratio called the blending factor ξ . In the blending scheme, the ξ value was determined by a trial-and-error method.

In order to verify the blending scheme, a benchmark study was made using Ar containing a small amount of metastable Ar* under 13.56-MHz RF E . As the results, the blending scheme was shown to be sufficiently accurate and very robust against coarse cell meshes (large $\Delta\epsilon$) especially at low E ; the EEDF, the EEPF, the mean electron energy, the drift velocity, and the ionization collision frequency are almost insensitive to $\Delta\epsilon$, whereas they significantly vary depending on $\Delta\epsilon$ in the conventional upwind scheme. As E increases, the differences between the upwind and blending schemes became small, where the ξ value obtained by the trial-and-error preprocess decreased as well.

Computational elapsed time was compared for the upwind and the blending schemes. Of course, the blending scheme is more complicated and needs longer elapsed time compared to the upwind scheme at the same $\Delta\epsilon$ resolution. However, considering the acceptable calculation error, a large value of $\Delta\epsilon$ was allowed in the blending scheme. This improved the overall efficiency of the PM calculation procedure, and can significantly reduce the total computation cost, which enabled an accurate and practical PM calculation under RF E . Thus, the key point of this work is very simple; the upwind scheme of electron flow calculation was replaced by the blending scheme in which the upwind and the central difference schemes were blended. This simple improvement in the PM calculation was found to give us great benefit in the reliability and efficiency.

The blending scheme has been built into a newly developed user-friendly computer software named BOSPROM, which enabled accurate and practical electron swarm analysis under

RF E . It was demonstrated that BOSPROM can successfully extract the characteristic behavior of RF nonequilibrium plasmas. This software can obtain exact solutions of the BE even in the extreme conditions where conventional calculations by the two-term approximation fail. Moreover, the computation time is much shorter than in MC calculations. In future, it is expected that many applications utilize the PM to obtain data of the EVDF and swarm parameters for reliable simulations of RF nonequilibrium plasmas.

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