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Numerical solutions to the weakly collisional plasma and sheath in the fluid approach and the reduction of the ion current to the wall

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Abstract

The plasma-sheath problem is solved numerically for the transition regime from collisionless to strongly collisional in both planar and cylindrical geometry. An improved frequency for ion-neutral momentum transfer collisions is introduced as a combination of the constant collision frequency and constant mean free path models. The model is correct in the limiting cases of collisionless and strongly collisional plasmas. The current density at the wall is calculated for a wide range of parameters and an analytic form $J = J_0 / (1 + \kappa L / \lambda)^{1/2}$ is found to describe the reduction of the flux, where J_0 is the ion flux for the collisionless case, L is the dimension of the plasma, λ is the ion-neutral mean free path and κ is a fitting parameter.

I. Introduction

There has been a recent increase of interest in plasmas and plasma sheaths in the transition regime from collisionless to strongly collisional (continuum).^{1,2,3,4} The transition regime means that the ratio of the ion-neutral momentum transfer mean free path λ and the size of the discharge L is finite and varies between $L/\lambda = 1-1000$. Within this regime the approximations in the limiting cases of collisionless or strongly collisional plasmas are invalid. The direct effect of collisions on the plasma is the reduced ion flux to the wall and also the lower average energy of ions striking the wall. Indirectly, however, collisions also affect other plasma parameters, such as the plasma potential and electron temperature. The particle balance equation is regularly applied in analytical as well as computational models of low pressure discharges. In the particle balance the generation rate of the plasma (ionization) is set equal to the rate at which ions are lost to the walls. The Bohm current flux^{5,6}, $0.5qn_0c_s$, is often used to describe the flux of ions to the wall, where q is the elementary charge, n_0 is the undisturbed plasma density and $c_s = \sqrt{T_e/m_i}$ is the ion sound speed with the electron temperature T_e in energy units. As collisions reduce the loss rate of ions to the wall, the plasma potential (relative to T_e) needs to increase to ensure the better confinement of the electrons.

The weakly collisional plasma-sheath problem has a kinetic and fluid approach. For the fluid model, Self and Ewald⁷ found the analytical solution in the plasma approximation. Numerical solutions to the problem were obtained e.g. by Forrest and Franklin,⁸ Ingold⁹ and Franklin and Snell.¹⁰ In these papers a model of constant collision frequency for momentum transfer has been applied. This collision model goes naturally

over to the constant mobility case that is valid for strongly collisional plasmas at high pressures. On the other hand, the constant mean free path model is physically more accurate at lower pressures. In the kinetic approach the ion density is calculated from the ion distribution function it is natural to apply the constant mean free path model to include collisions. The original kinetic theory of Tonks and Langmuir¹¹ has been extended by Riemann¹² to include collisions and solved for the plasma approximation in planar geometry. Wallschläger¹³ reported numerical solutions to the full plasma sheath problem for cylindrical geometry. Recently, Sternovsky and co-authors^{14,15} presented numerical results on the energy distribution of ions striking the wall and the reduced ion flux for both the planar and cylindrical cases. The above models assumed that ions are born cold. Bissell and Johnson¹⁶ have applied an ionization model in the collisionless case, where ions are born with a Maxwellian distribution.

Within the transition regime of plasmas, there is a smooth transition from constant collision frequency of ions near the center of the discharge to an approximately constant mean free path case in the sheath regions with high electric field. This transition is due to the finite temperature of ions. Near the center of the discharge the electric field accelerating the ions toward the walls is negligible. The fluid velocity u_d of ions is thus small compared to their thermal motion and collision frequency is independent of u_d . In the sheath region, on the other hand, the electric field accelerates the ions to velocities comparable or larger than the thermal speed and the collision frequency becomes proportional to u_d . This picture of transition from one collisional model to the other is consistent with the variation of ion mobility with the electric field intensity. For small electric fields the mobility is independent to the electric field, while for large fields it

decreases with increasing field.^{17,18} The smooth transition between the two regimes happens where the potential drop over a mean free path is comparable to the thermal energy of ions.

The purpose of this paper is to present a collision model for the hydrodynamic description of plasma-sheath problem that correctly describes the transition regime. The plasma-sheath equations are solved numerically with the emphasis being on the calculation of the flux of ions to the wall. This quantity is important for plasma processing applications and/or modeling plasmas with nonlocal electron kinetics.^{19,20,21,22} Although the ions are weakly collisional in the transition regime (the product of the pressure and dimension of the discharge is on the order of or lower than $pL \approx 1$ Torr cm) the distribution of electrons exhibits nonlocal characteristics if the energy relaxation length is larger than the dimension the plasma. Since the electron-neutral collision mean free path is approximately an order of magnitude larger than that of ion-neutral collisions,²³ nonlocal electron kinetics is valid through the transition plasmas with $L/\lambda \leq 1000$. For completeness we note, that for low pressure discharges the distribution of electrons is likely to deviate from a Maxwellian since the electrons from the tail of the distribution are lost to the walls.²⁴ In the present paper, however, this effect is not taken into account.

Two types of source functions are considered in the paper. In the proportional model it is assumed that the ionization is due to the plasma electrons and the rate of ionization is thus proportional to the electron density. In the homogenous ionization model it is assumed that the source function is independent of the position. Although proportional ionization is the prevailing model, there are numerous cases, where the

homogeneous model is more correct. Examples could be the hot filament discharges or the negative glow region of the DC glow discharge.²⁵ In these plasmas the ionization is due to minor population of high energy electrons (beam electrons).

The organization of the paper is as follows. In Sec. II the fluid equations of the plasmas-sheath and the collisional model are presented. The results from the numerical solutions are discussed in Sec. III and Sec. IV is the conclusion.

II. The collisional fluid model

The basic equations of the hydrodynamic plasma-sheath model are Poisson's, the continuity and the momentum equations:

$$\varepsilon_0 \nabla^2 \Phi(x) = -\frac{qJ(x)}{u_d(x)} + n_0 q \exp\left\{\frac{q\Phi(x)}{T_e}\right\}, \quad 1.$$

$$\frac{1}{x^\beta} \frac{d}{dx} (x^\beta n_i u_d) = R \quad 2.$$

$$\frac{u_d}{x^\beta} \frac{d}{dx} (x^\beta n_i u_d) + n_i u_d \frac{d}{dx} (u_d) + n_i u_d \nu(u_d) - \frac{q}{m_i} n_i E = 0 \quad 3.$$

where ε_0 is the permittivity of free space, Φ is the space potential, q is the elementary charge. The ion flux is $J_i = n_i u_d$ with u_d as the ion fluid velocity and $\beta = 0,1$ refers to

the planar and cylindrical case, respectively. The ionization models considered are homogeneous ionization rate, $R = R_0 = const$, and ionization proportional to the local electron density, $R(x) = R_0 \exp[q\Phi(x)/T_e]$.

The above physical model is similar to that of Franklin and Snell.⁴ The ion-neutral collisions are included with momentum transfer collision frequency $\nu_i(u_d)$. In the constant mean free path model the collision frequency is expressed in terms of the ion fluid velocity and the mean free path $\lambda = 1/n_n\sigma$, where n_n is the number density of neutrals. It is assumed that the collision cross section σ is independent of velocity. In the limit of high electric fields, $E\lambda \gg T_i$, where T_i is the ion temperature in energy units, the ion drift speed can be calculated by the integration of the ion velocity distribution function using kinetic theory²⁶ to obtain

$$u_d^K = \sqrt{\frac{2qE\lambda}{\pi m_i}}. \quad 4.$$

The above relation differs from the usual hydrodynamic result, $u_d^{HD} = \sqrt{qE\lambda/m_i}$, by a factor of $2/\pi$ in front of the mean free path λ . This means that in the fluid model the mean free path is reduced compared to the kinetic model and the corrected collision frequency to be used is

$$\nu(u_d) = \frac{\pi u_d}{2\lambda}. \quad 5.$$

Compared to the collision frequency $\nu(u_d) = u_d / \lambda$ used by Franklin and Snell⁴ the form in Eq. (5) is shown below to provide better agreement with the kinetic models.

The opposite limit, $E\lambda \ll T_i$, applies in the bulk of the plasma unless the mean free path is on the order of or larger than the size of the plasma. With this condition satisfied, the fluid velocity of ions is much smaller than their thermal speed. The collision frequency of ions is thus determined by their random thermal motion rather than their velocity as a fluid and thus $\nu = \sqrt{2}\bar{u} / \lambda$. In this relation $\bar{u} = \sqrt{8T_i / \pi m_i}$, and the collision frequency is independent of the fluid velocity. The factor $\sqrt{2}$ is due to the mutual motion of the ions and neutral assuming the same temperature for both species.²⁷ Wannier²⁸ has introduced the concept of collision frequency in the transition range as

$\nu(u_d) = \sqrt{[\nu_1(u_d)]^2 + [\nu_2(u_d)]^2}$, where ν_1 and ν_2 are the collision frequencies in the limiting cases. Following this approach the collision frequency of ions can be written as

$$\nu(u_d) = \frac{\sqrt{2\bar{u}^2 + \pi^2 u_d^2 / 4}}{\lambda}. \quad 6.$$

A similar collision frequency has been applied in a Monte Carlo model to calculate the mobility and diffusion of ions in low and high electric fields.²⁹ It is apparent that in the limit of zero ion temperature Eq. (6) is identical with the constant mean free path model. A finite ion temperature is required in order to properly describe the collision frequency in the transition regime. In the following the limits of validity are investigated. The ion flux in collisional plasmas is given by $\Gamma = \mu n E - D \nabla n$, where $\mu = q / m_i \nu$ is the ion

mobility and $D = T_i / m_i \nu$ is the diffusion coefficient. For Eq. (3) to be valid, the diffusive loss of ions has to be negligible compared to the ohmic term, i.e. $\mu m E \gg |D \nabla n|$. A very approximate estimate for the electric field and the density gradient can be made as $E \sim T_e / L$ and $\nabla n \sim n / L$, where L is the size of the plasma, giving a limiting condition on the ion temperature $\tau = T_i / T_e \ll 1$. The physical meaning of this relation is that for large ion temperatures (i.e. comparable to T_e) the flux of ions to the wall due to their thermal motion cannot be neglected. Similar reasoning can be used in the collisionless case. The random flux of ion due to the thermal motion has to be small compared to the sound velocity the ions gain as accelerated by the potential profile of the plasma. From here it follows that the $T_i / T_e \ll 1$ condition has to be satisfied also for the collisionless case. In this paper cases for $\tau \leq 0.1$ are considered.

Equations (1) to (3) can be integrated numerically using standard numerical techniques, for example the Runge-Kutta or Bulirsh-Stoer methods.³⁰ The integration starts close to the midplane, $x = 0$, and it is stopped at the wall, where the ion and electron fluxes are in balance. The random flux of electrons is given by

$$J_e(x) = n_0 \sqrt{T_e / 2\pi m_e} \exp[q\Phi(x) / T_e],$$

where m_e is the electron mass. It is convenient to

normalize the equations using variables: $X = x / \lambda_D$, $\varphi = q\Phi / T_e$, $U = u_i / c_s$, $N = n_i / n_0$,

$$G = R\lambda_D / n_0 c_s, \text{ and } \tilde{\nu} = \nu \lambda_D / c_s, \text{ where } \lambda_D = \sqrt{\epsilon_0 T_e / n_0 q^2}$$

is the Debye length. The

potential at $x = 0$ is chosen to be zero. The problem with $U_i = 0$ near $X = 0$ can be

overcome by approximating the potential profile in the vicinity of the $X = 0$ with the

form $\varphi(x) = -\alpha X^2$. Since $N_i \cong N_e \cong 1$ in this region, we find that $U_i \cong (\frac{1}{2})^\beta GX$. From

the momentum equation (3) the rate of ionization can be calculated as $G = \sqrt{\alpha}$ and $G = \sqrt{8\alpha/3}$ for the planar and cylindrical symmetries, respectively. The numerical calculations presented are for an electron-proton plasma.

III. Numerical results and discussion

First, the numerical results for the collisionless case have been investigated in the large plasma limit in order to test the numerical code against previous analytical or numerical results. The values of the ion flux to the wall for $L/\lambda_D \rightarrow \infty$ are listed in Tab. I. for the cases investigated. The results for planar geometry agree with the well known Bohm result. The proportional ionization case in cylindrical symmetry is in agreement with the result $J_w = 0.419n_0c_s$ given in Refs. [6,7]. There appears to be no reference for the homogeneous ionization case in cylindrical geometry. The ion flux to the wall in the kinetic approach³¹ $J_w = 0.489n_0c_s$ is in close agreement with the fluid result for the planar case. In cylindrical geometry the discrepancy is larger as the kinetic models^{13,15} gave $J_w = 0.415n_0c_s$ and $J_w = 0.380n_0c_s$ for the homogeneous and proportional ionization models, respectively.

For the constant mean free path case ($T_i = 0$) the results were compared to those of Franklin and Snell⁴ for planar geometry, proportional ionization and argon gas. The agreement between the results was correct to the precision given in Ref. [4]. It is, however, necessary to note that the collision model of Franklin and Snell used a collision frequency $\nu(u_d) = u_d/\lambda$, which differs from the collision frequency in Eq. (5) by a

factor of $\pi/2$. The magnitude of difference between the two collisional models is indicated in Fig. 1. The numerical results from the presented fluid model were compared to those from a kinetic model reported by Sternovsky et al.¹⁴ and Sternovsky¹⁵ for the planar and cylindrical geometries. The figure shows that the kinetic results are in better agreement with the fluid results when a collision frequency from Eq. (5) is used. Figure 1 shows fluid calculations for $L/\lambda_D = 1000$ and $L/\lambda_D = 252.8$. The calculations for the latter case were done for a direct comparison with the data from the kinetic model.

It was found that the reduction of the ion flux can be accurately approximated for $T_i \rightarrow 0$ with the analytic formula

$$J = \frac{J_w(L/\lambda_D)}{\sqrt{1 + \kappa L/\lambda}}, \quad 7.$$

where $J_w(L/\lambda_D)$ is the collisionless ion flux for a plasma of dimension L/λ_D , and κ is a fitting parameter. The value of $J_w(L/\lambda_D)$ is within few percent of the ion flux in the limiting case $L/\lambda_D \rightarrow \infty$ for plasmas¹⁴ $L/\lambda_D > 100$. The numerical calculations were done for a plasma of dimension $L/\lambda_D = 1000$ with the mean free path varied from the collisionless case up to $L/\lambda = 1000$. The value of the fitting parameters for the different cases is shown in Table I. It is important to note that the value of κ is independent of L/λ_D and thus the effect of finite plasma dimension is incorporated in $J_w(L/\lambda_D)$ only. For $T_i = 0$, the analytic approximation is accurate within about 1-2% on average with a maximum error of 6% for the investigated parameter range.

The effect of finite ion temperature on the ion flux is shown in Fig. 2. The flux decreases with increasing ion temperature because of the increase of the collision frequency (see Eq. 5) even though the mean free path remains the same. The significance of the finite temperature clearly increases with increasing collisionality (L/λ) of the plasma. It is also possible to fit Eq. (7) on the data for $T_i > 0$, although the accuracy of the fit is limited. Listed in Table I are the values of the fitting parameter for $T_i/T_e = 0.003$, and $T_i/T_e = 0.1$ that are valid with better than 10% accuracy for $L/\lambda \leq 100$ and $L/\lambda \leq 10$, respectively.

The plasma for finite ion temperature and large L/λ approaches Shottky's strongly collisional result [6] originally presented for the positive column of a DC glow discharge. Figure 3 shows the change of the potential profile with increasing collisionality in cylindrical geometry and proportional ionization. In the limit of large plasma $L/\lambda_p \rightarrow \infty$ and strong collisionality (continuum) it is valid that $L\sqrt{\nu R_0} \rightarrow 2.405$. Figure 4 shows that this limit is in fact approached.

IV. Conclusions

An improved collisional plasma-sheath model was presented in the hydrodynamic approach. The model incorporates the limiting cases of constant collision frequency, valid in the bulk of the plasma, and constant mean free path valid in the sheath region. The transition between the two cases is due to the small, but finite ion temperature. The model of the constant mean free path case was corrected by a factor of $\pi/2$ in order to bring the fluid solution closer to physically more complete kinetic plasma model. It was

shown that the ion flux to the wall decreases with increasing ion temperature. This is due to the increased collision frequency with the increasing thermal motion of ions. The collisional plasma-sheath model provides the expected results in the limiting cases.

The numerical calculations were performed in order to determine the collisional reduction of the ion flux to the wall. A sufficiently accurate analytic approximation was found and is useful for modeling weakly collisional plasmas in the transition regime. Robertson and Sternovsky³² have recently published a model that calculates the plasma parameters (electron temperature, plasma potential) of a low-density hot-filament discharge from first principles, i.e. the particle and energy balance of electrons and ions. It is shown in a subsequent paper³³ that the validity of the model can be extended into the weakly collisional parameter range by including the effect of reduced flux of ions to the wall.

Although the numerical solution of the presented collisional fluid model also yields the potential (and hence the electric field) at the wall, the significance of this parameter is limited for most plasmas of interest. As discussed above, the weakly collisional regime coincides with the parameter range ($L/\lambda = 1-1000$), where nonlocal electron kinetics is valid. In reality, the electron distribution function of most nonlocal plasmas exhibit multiple populations of electrons and/or incomplete tail of a Maxwellian velocity distribution. The plasma potential is thus going to depend also on the form of the electron energy distribution function. On the other hand, the ion flux to the wall is generally only a function of the temperature of the electron population trapped by the plasmas potential.

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Table I. The fitting parameters for the ion flux reduction for different sheath models. The $\beta = 0, 1$ corresponds to planar and cylindrical geometry, respectively.

Model	$J_W / n_0 c_s$ ($L \rightarrow \infty$)	κ $T_i = 0$	κ $T_i = 0.03$	κ $T_i = 0.1$
$\beta = 0$, homogeneous.	0.5	0.293	0.33	0.70
$\beta = 0$, proportional	0.5	0.351	0.39	0.82
$\beta = 1$, homogeneous	0.439	0.220	0.26	0.58
$\beta = 1$, proportional	0.419	0.284	0.33	0.74

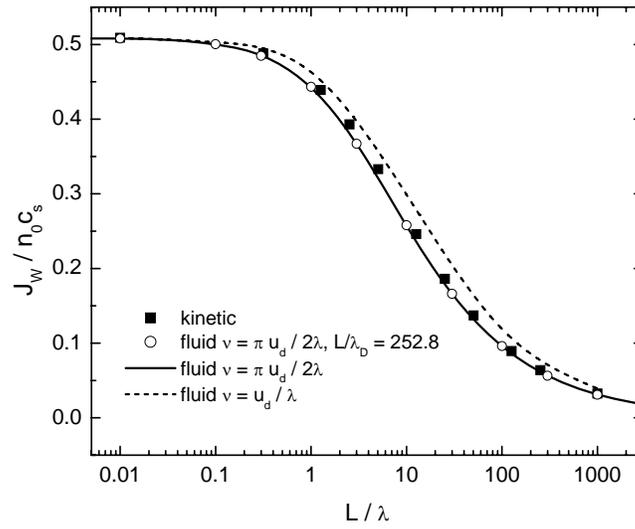


Fig. 1. The reduction of the ion flux to the wall with increasing collisionality for $T_i = 0$ (constant mean free path). The curves are calculated for the planar case ($\beta = 0$), plasma size $L / \lambda_D = 1000$ and homogeneous ionization with two collisional frequency models. The full squares are calculated from a kinetic model for $L / \lambda_D = 252.8$ (Ref [14]). The open circles are from a fluid model for $L / \lambda_D = 252.8$ and have been scaled vertically to have the same flux for $L / \lambda \rightarrow 0$.

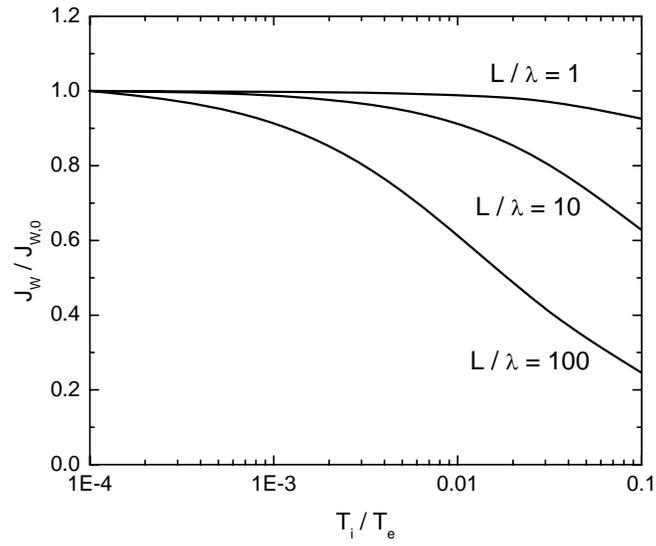


Fig. 2. The decrease of the ion flux to the wall with increasing ion temperature. The calculations are for plasma size $L = 1000\lambda_D$, planar geometry and ionization proportional to the electron density. The three curves are for different collisionality of the plasma.

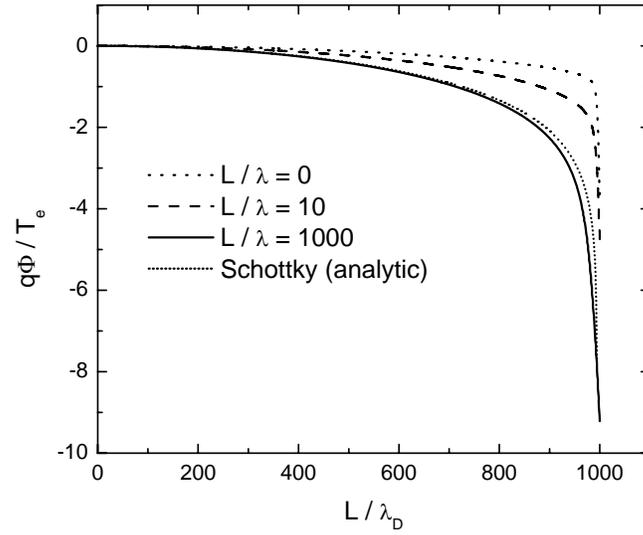


Fig. 3. The change of the potential profile with increasing collisinality. The calculations are for cylindrical geometry, proportional ionization, plasma dimension $L = 1000\lambda_D$, ion temperature $T_i/T_e = 0.1$ and various mean free paths. The short-dotted line is the analytic result from the Schottky theory. The curves end at the potential of the wall.

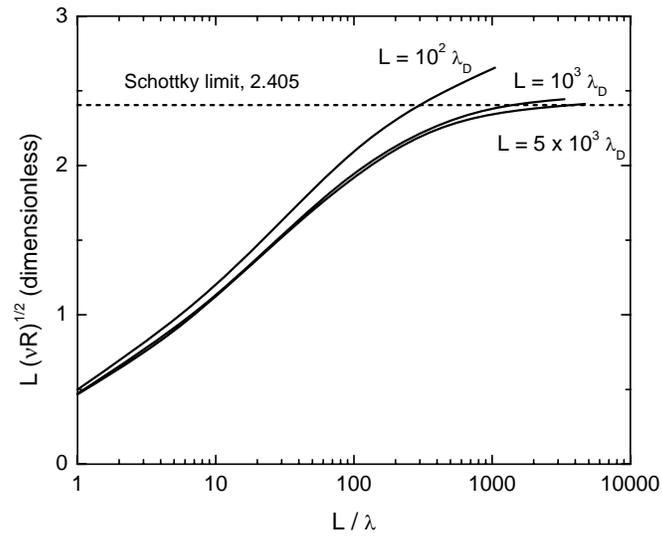


Fig. 4. The collisional plasma-sheath model approaches the Schottky limit for strong collisionality and large plasmas. The calculations are done for cylindrical geometry, proportional ionization, and $T_i/T_e = 0.1$.