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Modelling of plasma momentum transference to side-walls by neutral particles

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Abstract

Monte Carlo modelling of plasma extinction by neutral particles requires energy and momentum sinks to be determined with sufficient statistical significance. We focus on this aspect using calculations of an idealized 1D plasma–gas interface with the Eirene code. A novel non-linear version including self-collisions amongst neutral particles is also applied to admit gas viscosity. It emerges that statistically significant momentum losses often cannot practicably be determined, even at modest plasma temperatures (~ 10 eV), using conventional collision-estimator techniques. Gas viscosity effects also tend to inhibit extraction of plasma momentum and hinder extinction. Certain possibilities to improve numerical methods are mentioned.

Keywords: Divertor plasma; Monte Carlo simulation; Momentum sink; Detached plasma

1. Introduction

In an ignited next-step tokamak, conventional high recycling divertor operation would probably incur severe plasma loads on target surfaces, causing their endurance to be unacceptably low [1,2,5]. An alternative proposal is therefore largely to absorb the diverted plasma in a neutral gas target, which then mitigates the burdens by spreading them over greater side wall areas. Such 'detached' states were first proposed on the basis of simple 1D pictures [2–4] where the principles of extinguishing a scrape-off plasma were indicated. More elaborate explorations [5,6] for specific tokamak conditions have followed using detailed numerical models of edge transport, but now their intricacy tends to complicate identification both of basic features and of limitations of the method itself. An instance is that for Monte Carlo resolution of neutral particle behaviour, its statistical estimates of related sources and sinks have to achieve an adequate *significance level.*

A dynamic process of plasma detachment is governed by lateral transference of plasma *energy* and longitudinal *momentum* to walls by neutral particles. Essentially, a compromise regime must be found in which events such as atomic charge-exchanges with ions are frequent enough to collect their momentum, but subsequent atomic mean-free paths are long enough for them to reach the walls. To focus on these fundamental effects, and statistical significance of loss terms, an idealized plasma–gas problem has been studied using the Eirene Monte Carlo code [7]. Efficiency of plasma depletion and amenability to statistical calculation are investigated over ranges of conditions liable to be met in full edge modelling of emerging detachment. Importantly for a gas target, usual linear Monte Carlo treatment neglects collisions between neutral particles themselves, whereas they are likely to be prolific at least in the region between the plasma rim and walls, affecting associated transport properties. A novel *non-linear* formulation of Eirene is able for the first time to include these self-interactions as well [8]. A preliminary

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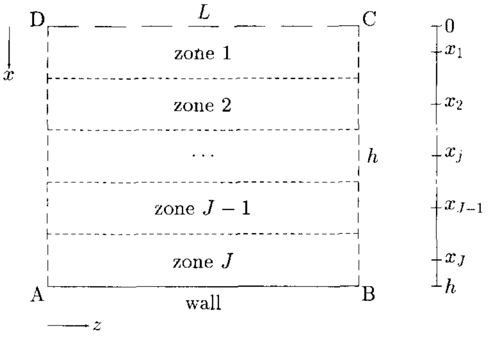


Fig. 1. Geometry of slab problem.

application is made to test the influence of finite gas viscosity on plasma extinction.

2. Idealized problem

We consider a simple slab geometry, infinite in the normal (y) and along-field (z) directions, but with specified profiles of a pure deuterium plasma in a number of consecutive layers j ($1 \le j \le J$) across the field (x). A wall, taken to be composed of carbon at 300 K, bounds the outermost zone $j = J$ (see Fig. 1). Deuterium molecules at this same temperature are injected at a uniform source rate density ($\frac{1}{2}S_0$ m^{-2} s^{-1}) from the wall. A symmetric, enclosed system is then obtained by making the interior boundary ($x = 0$) specularly reflecting, so that calculations address one half of a perfectly symmetric column between two identical parallel walls, reminiscent of a so-called slot divertor arrangement. Our innermost zone $j = 1$ hence corresponds to the centre of the plasma stream.

A static, test-particle treatment is adopted, namely steady sources and sinks are computed for a given, unresponding plasma background. This corresponds technically to the completely converged, steady-state situation with a full, mutually consistent plasma–gas edge model [9]. In other words, an equivalent position is reached asymptotically in coupled transport simulations iterating [9] between Eulerian plasma and Monte Carlo gas codes. We further assume ideal absorbtion of longitudinal momentum (v_z) of any neutral particles scattered back onto the wall from the plasma, so that on average they are reemitted again with $v_z = 0$. This provides for the most favourable limiting estimates of dynamic neutral–particle friction.

To reduce the number of variables, we take $T_e = T_i \equiv T$. Plasma profiles are thereafter defined in a chosen number of zones $1 \le j \le j_p \le J$ as two-parameter functions:

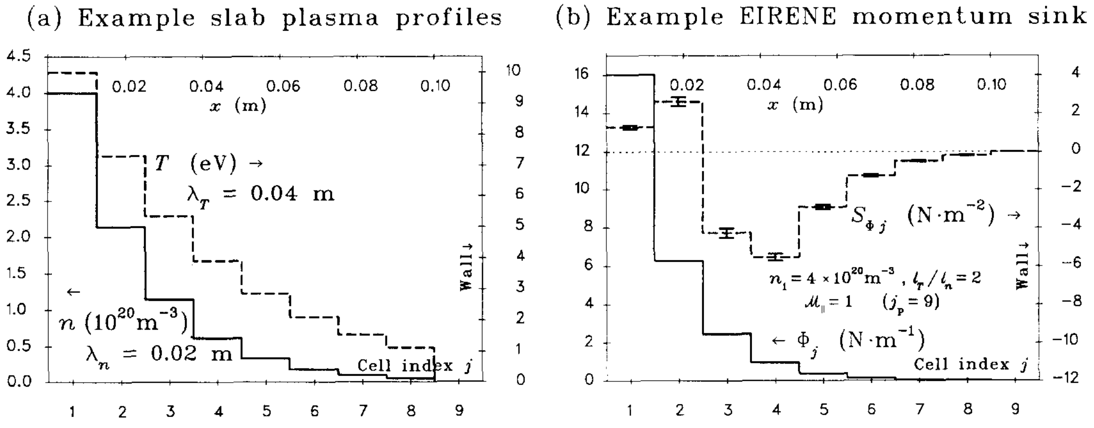
$$n_j = \Theta_j(n_1, l_n); \qquad T_j = \Theta_j(T_1, l_T),$$

where n_1; T_1 are their central peak values and l_n; l_T their cross-field decay lengths, while $\Theta_j(a, b)$ is a general two parameter discretized exponential designed to fall exactly to zero by zone $j = j_p$, viz:

$$\Theta_j(a, b) \equiv a\left(\frac{\mathrm{e}^{-(x_j - x_1)/b} - \mathrm{e}^{-(x_{j_p} - x_1)/b}}{1 - \mathrm{e}^{-(x_{j_p} - x_1)/b}}\right).$$

An outer plasma-free space in zones $j_p \le j \le J$ (here denoted 'void') is consequently introduced between the plasma and wall. For linear Monte Carlo calculations with no neutral particle–neutral particle interactions, this is trivially represented by just a single zone ($j_p = J$), as they merely fly freely across it. However, it becomes more significant in non-linear Eirene cases, as discussed later. Resulting slab profiles are exemplified in Fig. 2(a), in which $n_1 = 4 \times 10^{20}$ m^{-3}; $l_n = 2$ cm; $T_1 = 10$ eV; $l_T = 4$ cm; $j_p = 9$; and the plasma rim lies at $\frac{1}{2}(x_{j_p} + x_{j_p-1}) = 10$ cm measured from the centre of the column ($x = 0$).

Flow along the slab is defined by a uniform parallel Mach number $\mathscr{M}_\parallel$, i.e. $v_{zj} = \mathscr{M}_\parallel\sqrt{2T_j/m_i}$, plus $v_{yj} = v_{xj} = 0$. If each zone has respective cross-field (x) thickness d_j (where $x_j = \frac{1}{2}d_j + \sum_{k=1}^{k=j-1} d_k$), total plasma fluxes of ions,


(a) Example slab plasma profiles

(b) Example EIRENE momentum sink

Fig. 2. (a) Example slab plasma profiles, (b) example Eirene momentum sink.

Table 1
Plasma-gas interactions included

$e+D_2 \rightarrow e+2D$	(dissociative excitation)	(i)
$e+D_2 \rightarrow 2e+D+D^+$	(dissociative ionization)	(ii)
$e+D_2 \rightarrow 2e+D_2^+$	(molecular ionization)	(iii)
$e+D_2^+ \rightarrow e+D+D^+$	(ion dissociation)	(iv)
$e+D_2^+ \rightarrow 2e+2D^+$	(ion ionization)	(v)
$e+D_2^+ \rightarrow 2D$	(dissociative recombination)	(vi)
$e+D \rightarrow 2e+D^+$	(two-body ionization)	(vii)
$D^+ +D \rightarrow D+D^+$	(charge exchange)	(viii)
$D^+ +D \rightarrow D^+ +D$	(atomic elastic collision)	(ix)
$D^+ +D_2 \rightarrow D^+ +D_2$	(molecular elastic collision)	(x)

momentum and energy per unit depth in the normal (y) dimension are thus given by

$$\Gamma_i = \sum_{j=1}^{j=j_p-1} d_j n_j \mathcal{M}_\parallel \sqrt{\frac{2T_j}{m_i}} \left(\frac{1}{\mathrm{s\,m}}\right);$$

$$\Phi = \sum_{j=1}^{j=j_p-1} d_j n_j \mathcal{M}_\parallel^2 2T_j \left(\frac{\mathrm{N}}{\mathrm{m}}\right);$$

$$Q^{\mathrm{convect}} = \sum_{j=1}^{j=j_p-1} d_j n_j \mathcal{M}_\parallel \left(5T_j + \mathcal{M}_\parallel^2 T_j\right) \sqrt{\frac{2T_j}{m_i}} \left(\frac{\mathrm{W}}{\mathrm{m}}\right).$$

Energy transport is purely convective, there being no longitudinal gradients.

Lastly, dominant plasma–neutral particle interactions included are listed in Table 1. Reactions (viii) (charge exchange), (ix) and (x) (elastic scattering) are those capable of transferring plasma momentum to neutral particles, which may then travel back to, and deposit it onto, the walls. Discrimination of atomic charge-exchange and elastic scattering is computationally convenient, although these reactions could not be distinguished practically.

3. Depletion efficiencies (plasma momentum and energy)

Since all neutral particles injected are eventually ionized, total ion source rate per unit transverse ($y \cdot z$) area satisfies $S_i = S_0$. A *particle-doubling*, or refuelling, length may therefore be defined:

$$L \equiv \Gamma_i / S_0 \ (\mathrm{m}),$$

over which as many particles are added as ions are streaming along the slab. Similarly integrating total parallel momentum S_Φ (N m^{-2}) and energy S_Q (W m^{-2}) sinks derived per unit transverse area, equivalent *extraction* lengths may be inferred:

$$L_\Phi \equiv \Phi / |S_\Phi| \ (\mathrm{m}); \qquad L_Q \equiv Q^{\mathrm{convect}} / |S_Q| \ (\mathrm{m}).$$

Indicative dimensionless extinction lengths may thus be deduced (L_Φ / L_n); (L_Q / L_n). Alternatively, reciprocals of these numbers indicate normalized plasma momentum and energy removal per ionization, i.e.,

$$(|S_\Phi|/S_0)/(\Phi/\Gamma_i) = (L_n/L_\Phi);$$

$$(|S_Q|/S_0)/(Q^{\mathrm{convect}}/\Gamma_i) = (L_n/L_Q).$$

Viability of detached divertor operation depends on these efficiencies (L_n/L_Φ); (L_n/L_Q) being sufficiently large, so that each neutral particle added performs enough momentum and energy transfer to the walls before being lost by ionization [3]. Equivalently, their inverse lengths (L_Φ/L_n); (L_Q/L_n) have to be small enough for a practicable divertor design.

4. Linear Monte Carlo results (no neutral particle self-interactions)

A possibility to extinguish a cool plasma efficiently is demonstrated in a case taking $n_1 = 2.5 \times 10^{19}$ m^{-3}, $l_n = 2$ cm, plus a nearly constant low temperature, provided by $T_1 = 2$ eV, $l_T = 100$ m. Normalized removals per neutral particle are found to be $(L_n/L_\Phi) \approx 150$, $(L_n/L_Q) \approx 180$, for $\mathcal{M}_\parallel = 0.1$ or 1.0. Such effectiveness occurs below some threshold [3,10] temperature $T_c \approx 5$ eV, owing to preponderance of plasma momentum collecting events (charge exchange (viii) elastic scattering (ix) and (x)) over ionizations. In full edge modelling calculations of the *approach* to divertor detachment, however, it is necessary also to ensure a valid treatment of more opaque conditions prior to reaching this amenable regime. Note that energy sinks S_Q then actually consist substantially of ionization losses, which persist in the plasma column as potential energy of new electron–ion pairs. Volume recombinations would additionally be needed to avoid concentrated loading still of some end surface.

To consider plasma quenching, peak density n_1 has been varied for a decay-length of $l_n = 2$ cm, a peak temperature of $T_1 = 10$ eV, and decreasing relative thickness of the temperature profile (l_T/l_n). Note that T_j typically remains $\lesssim 5$ eV over most of the slab. These variations symbolize the possible adjustment of a diverted plasma column subjected to cooling by radiation and enveloping neutral particles; namely, contraction of its hotter centre, while there is some increase in the density.

A sample result is depicted in Fig. 2(b), where again $n_1 = 4 \times 10^{20}$ m^{-3}, $(l_T/l_n) = 2$, and $\mathcal{M}_\parallel = 1$. Approximate 95% confidence intervals are shown on the momentum sink $S_{\Phi j}$ in each zone, seen here to be well determined. In particular, though, $S_{\Phi j}$ is seen to be *positive* in the core of the slab ($j = 1, 2$), where most of the streaming plasma momentum and energy is concentrated. Neutral particles hence may acquire momentum by scattering in the outer layer of the plasma, and redeposit it upon ionization in the centre (locally increasing the momentum, though probably lowering the velocity). This case illustrates a capability, newly clarified in our studies, for neutral particles to transport plasma momentum *inwards* across the column, oppositely to the direction desired. Such a mechanism has, for example, recently been suggested as contributing to very intense divertor bands observed in the ALCATOR-CMOD experiment [11]. In such circumstances, ultimate extraction of momentum to allow detachment to occur would have to rely upon plasma diffusive and transverse viscous processes carrying it out into the periphery, from where neutral particles would be able to remove it (to the walls).

A set of 10^5 Monte Carlo test-flights hake been propagated here and in all subsequent linear Eirene calculations. To assess statistical significance of (L_Φ/L_n) values obtained, each case has been repeated 6 times with different random number sequences, then means and variances estimated. Correlations between errors of separate components in losses are thereby most easily accommodated. Results with corresponding approximate 95% confidence intervals are summarized in Fig. 3. Attention is focused on momentum losses, since by their vector nature they are inherently more difficult to determine statistically. Related moments are estimated by accumulating contributions individually proportional to a relative motion vector which can be oriented arbitrarily in a 3D velocity space. The time-independent treatment used also allows maximum accuracy for collision-estimator based quantities, as they are presently implemented [7,8] for some relevant terms in Eirene.

Momentum sinks remain strong and adequately determined at lower density (Fig. 3), for either $\mathcal{M}_\parallel = 0.1$ or 1.0. As the density rises, however, they become weaker, owing partly to a rise in the relative rate of ionization. Modification with decreasing (l_T/l_n) suggests also that the central plasma tends to be screened by collisions in the cooler periphery, making it more difficult for neutral particles to penetrate into and deplete the main plasma stream as its temperature profile narrows. It is especially apparent that statistical estimates of losses simultaneously become more uncertain. For narrower temperature profiles and higher densities, error bars tend to span the zero line, the more so for lower plasma flows $(\mathcal{M}_\parallel)$. Formally these estimates are not discriminated from a null hypothesis that they are zero (infinite momentum transfer per atom), i.e. equivalent to their being completely *undetermined*. Thus a range of plasma properties, at modest temperatures, is implied, for which Monte Carlo momentum sinks cannot practicably be evaluated. This may limit full edge modelling applications, when in practice such conditions might be encountered. Certain improvements in methods aimed at remedying the situation are suggested below.

5. Non-linear Monte Carlo trial (neutral particle self-interactions included)

To transfer diverted fluxes onto the walls, scattered neutral particles must escape not only from the plasma but also across the surrounding void space. Here collisions

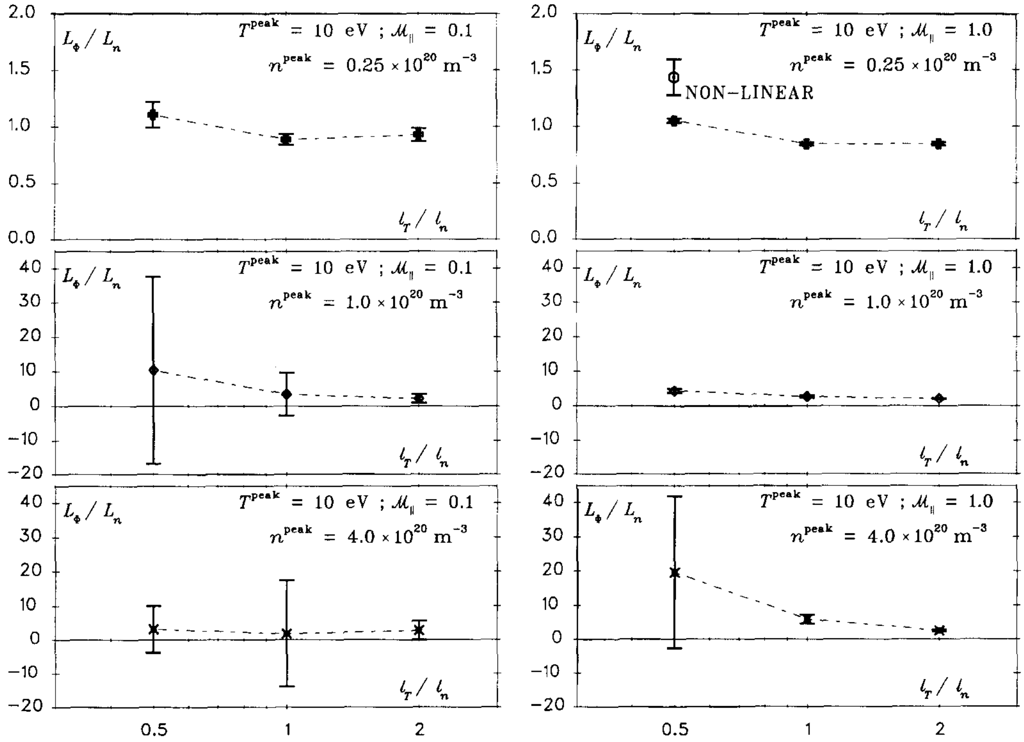


Fig. 3. Momentum removal for varying slab plasma properties.

amongst *themselves* will tend to degrade the efficiency of transmission [10], as free kinetic propagation develops into viscous transport. A novel extension of Eirene now includes these elastic self-collisions too by iterative Monte Carlo solution of a set of coupled BGK equations [8]. These involve notional neutral background species, which are progressively relaxed according to successively estimated distribution functions. Final converged solutions can overall approach any consistent distributions, e.g. potentially departing arbitrarily from local thermalization or laminar flow conditions.

In addition to those reactions listed in Table 1, elastic collisions are permitted between atoms, molecules, and atoms and molecules. Freedom exists with BGK couplings within a binary mixture to choose their rate coefficients so as to match three selected transport coefficients [8]. For present purposes, one is particularly taken as the viscosity of (thermal) molecular deuterium.

Up to turbulent modifications, viscous effects are governed [10] by the associated Knudsen number $K \equiv \lambda_0/d$, where λ_0 is the (atom) mean-free path and d the plasma rim to wall distance. Preceding linear Eirene cases default K to infinity, while a fluid neutral gas would imply $K \ll 1$. As mentioned above, in the former approximation of non-interacting neutral particles, the void between plasma and wall consequently exerts no influence on results, and the input source rate density S_0 is eliminated by considering normalized extinction lengths (L_{Φ}/L_n), (L_Q/L_n). In non-linear Eirene calculations, however, a combination of d and S_0 will determine the gas density and Knudsen number within the void space, and so control behaviour. We study first an instance with details adjusted to yield an intermediate figure $K \lesssim 1$. Note the void has now also to be divided into a number (10) of discrete zones, in order to resolve variations in the gas.

Again 6 calculations with different statistics are taken, each performing 25 iterations of BGK integrations using $\geq 10^4$ test-flights. Parameters used are $n_1 = 2.5 \times 10^{19}$ m^{-3}, $(l_T/l_n) = 1/2$, $\mathscr{M}_{\parallel} = 1$, and the resulting (L_{Φ}/L_n) is superimposed on Fig. 3. A significant reduction in the efficiency of momentum removal is seen compared to the previous free-streaming value ($\sim 40\%$ greater length). A second series of 6 runs (each 25 iterations, $\sim 4 \times 10^4$ test-flights) retaining the same plasma but adjusting S_0 to lower Knudsen number further to $K \lesssim 0.1$ finds nearly the same (L_{Φ}/L_n) within comparable error bars, suggesting the influence of specified gas self-collisions here is saturating [10] at this level. It is hence seen that viscous inhibition of plasma momentum transfer to walls could affect next-step divertors, depending on the Knudsen number to be expected [10].

6. Discussion

Idealized Monte Carlo calculations of neutral gas impinging on a plasma column corroborate efficient transfer of its momentum to side-walls, if it is cool enough ($\lesssim 5$ eV) or low enough in density. At higher densities and central temperatures, screening of neutral particles by the outer layers tends to impede depletion of the main plasma flow. Lengths for absorbtion increase, and statistical computation of momentum losses in particular can lose adequate significance. This may be important in related edge modelling of divertor detachment, developing through such conditions. Neutral particle self-collisions may also inhibit momentum transfer and so hinder extinction.

Various numerical techniques could be invoked to improve statistical accuracy, such as use of track-length rather than collision estimator methods for momentum sinks. Uncertainties might also be reduced by relating individual contributions in statistical sums more directly to expected averages [8]. In coupled plasma–gas edge models, no account is yet taken of confidence levels of Monte Carlo source and sink terms, local values of which are incorporated into the next plasma step whether or not they are significantly determined. Properly, those local estimates not distinguished at some required level (e.g. 95% confidence) explicitly from zero fail against this null hypothesis and cannot be regarded as being resolved. They should therefore be rejected, i.e. replaced with zero. A final global rescaling could still ensure particle conservation. Filtering Monte Carlo sources in such a manner should help to eliminate their least certain parts, so reducing noise and perhaps expediting achievement of jointly consistent solutions.

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