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Non-linear effects on neutral gas transport in divertors

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Abstract

The effects of neutral particles on the condition of the plasma edge play a key role in divertor and limiter physics. In computational models they are usually treated in the linear test particle approximation. However, in some divertor concepts a large neutral gas pressure is required in the divertor chamber to provide sufficient neutral–plasma interaction in the plasma fan (momentum removal and energy dissipation) and to permit adequate pumping performance. In such regimes viscous effects in the neutral gas may become relevant. We have extended the EIRENE code to solve the Boltzmann equation with a non-linear BGK-model collision term added to its standard linear collision integrals. The linear in-elastic collision integrals are reconsidered with respect to volume recombination and momentum removal efficiency from the plasma. The numerical procedure in the EIRENE Monte Carlo code is outlined. A simple test application (Couette flow) shows that the procedure works properly. First numerical studies have been carried out and the results are discussed.

Keywords: ITER; Momentum sink; Neutral transport; Monte Carlo simulation; Atomic physics

1. Introduction

Combined plasma-fluid and neutral particle kinetic codes are widely used for interpretative and predictive plasma edge modeling. A major effort throughout the world, partially triggered by the critical ITER divertor design issue, has led to the development and the application of plasma-fluid transport codes linked to either fluid neutral descriptions or kinetic linear (often Monte Carlo-) models. [1]

Whereas in most current experiments the linear model (i.e., the neglect of neutral–neutral collisions) appears to be adequate, due to their increased size, the next generation devices may well operate in the transition flow regime for neutral gas transport in the divertor and vacuum system. Under such conditions, apart from improved pumping performance, the effective momentum removal from the divertor to the side walls may be affected.

The sensitivity of divertor plasma conditions to momentum removal (friction between ions and neutrals) is most clearly visible by considering 2-point models with correction factors 'f' relating upstream ('u') to downstream ('t'-target) conditions [4]. For example, the global parameter f_{fric} has been introduced to account for friction and other volumetric losses arising in the pressure balance. It is found that the target plasma conditions n_t, T_t and the sputtered impurity flux $\Phi_{\mathrm{imp}}^{\mathrm{in}}$ are extremely sensitive to the rather uncertain parameter f_{fric}, and hence perhaps unpredictable. This is a consequence of the assumption of extremely high recycling within the divertor SOL inherent in this two point model. A low recycling SOL is much better predictable, but is perhaps not compatible with fusion reactor environments.

In this paper we will discuss physical and numerical issues related to the parameter f_{fric}. In Section 2 we discuss processes relevant to the momentum transfer from the plasma to the neutrals, and in Section 3 a procedure to study the transport of momentum through the neutral gas to the solid divertor structures under transition flow regime

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[1] For the code system used here (B2-EIRENE code): First release and ITER applications, see Ref. [1]. Many revisions since then by various groups e.g., Ref. [2]. Concept of code package described in Ref. [3].

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conditions. In the final Section 3.2 this is applied to an ITER-size divertor configuration and vacuum conditions such that 'Knudsen numbers' (see below) of order unity result.

2. Recombination, momentum removal

Recently the relevance of plasma recombination in the volume has received renewed attention [5]. The role of vibrationally excited molecules ($H_2(v)$) in triggering enhanced recombination efficiencies has been pointed out long ago, probably first in Ref. [6]. It was recently estimated again in Ref. [7], where large enhancement factors

$$n_{H_2}\langle \mathrm{rec}\rangle^{\mathrm{mol}}/n_{H^+}\langle \mathrm{rec}\rangle^{3+r}$$

over three-body recombination (up to 30 and more) are reported at low temperature (1–4 eV) and high density ($n_e = 10^{21}$ (1/m^3)). Here n_{H_2} and n_{H^+} are the molecule density and the hydrogen ion density, respectively, and $\langle \mathrm{rec}\rangle^{\mathrm{mol}}$ and $\langle \mathrm{rec}\rangle^{3+r}$ are the recombination rate coefficients for 'molecular activated' recombination and for three-body plus radiative recombination, respectively.

Two channels contributing to $\langle \mathrm{rec}\rangle^{\mathrm{mol}}$ are considered in Refs. [6,7]:

(1) $e + H_2(v) \rightarrow H_2^- \rightarrow H + H^-$, followed by

$H^+ + H^- \rightarrow H + H^*$

(2) $H^+ + H_2(v) \rightarrow H + H_2^+$, followed by

$e + H_2^+ \rightarrow H + H^*$

In both channels one electronically excited H-atom is produced. Within the concept of collisional radiative models this can either decay to ground state or be re-ionized, by chains of collisional radiative processes. Only in the former case do the above two channels qualify as 'recombination', and the branching ratio between the two possibilities is critical.

If this branching is taken into account within the frame of a collisional radiative model for hydrogen atoms (e.g., Ref. [8]), one finds that the conversion of H_2^+ into $H^+ + H$ in process 2 is about 50–100 times faster than the true recombination into ground state. This results in much smaller enhancement factors for recombination than would be expected without full account of collisional and radiative transitions between the various electronic states of atoms and molecules.

Similar arguments apply to the first channel.

We consider a combined collisional radiative model for molecules and atoms based on the work of Sawada and Fujimoto [8], supplemented by a collisional (and not radiative) model for vibrational excitation of molecules [9]. This model solves in a standard 'collisional radiative procedure' for reduced population coefficients of excited H atoms ($n = 2, \ldots, 30$), vibrationally excited H_2 molecules ($v = 1, \ldots, 14$) and electronically excited H_2, with 30 singlet and 29 triplet states, given the densities of ground state H, H_2, H_2^+ and H^+. From those coefficients, effective (plasma density dependent) rates for e.g., H^-, H_2^+ production, recombination, dissociation, etc., can be derived.

In Fig. 1 the resulting recombination rate coefficients $\langle \mathrm{rec}\rangle^{\mathrm{mol}}$ (split into channel 1 and 2) and $\langle \mathrm{rec}\rangle^{3+r}$ are shown, once for a case with no re-absorption of radiation, and once for the 'Lyman-opaque' extreme case (radiative transition $2 \rightarrow 1$ in the H-atom forbidden). The two rate coefficients $\langle \mathrm{rec}\rangle^{\mathrm{mol}}$ have been divided by ratios $n_{H_2}/n_{H_2^+}$ and n_{H_2}/n_{H^-}, respectively, such that the corresponding rates are obtained by multiplying both rate coefficients by $n_{H_2} \cdot n_{H^+}$ (a procedure justified by the short lifetime of H_2^+ and H^-).

Due to the above mentioned branching for the fate of the excited H-atom and the fact that the vibrational distribution of molecules is independent of electron density here, the strongest effect of $\langle \mathrm{rec}\rangle^{\mathrm{mol}}$ is to be expected at low electron densities. At the high electron densities almost all excited H^*-atoms produced in either channel 1 or 2 are re-ionized by ladder like (multi-step) processes before they have a chance to reach the ground state.

In the few eV electron temperature range and for $n_e = 10^{21}$ the recombination rates are strongly (roughly a factor 10) reduced by turning from the Lyman transparent to the Lyman opaque case, because the above mentioned transition into ground state is further aggravated.

This, and the rather modest enhancement factors of order unity (2–4) obtained for a ratio $n_{H_2}/n_{H^+} = 0.1$ differ significantly from the results obtained in the two papers cited in Ref. [7], where, in particular, much larger enhancement factors are found, but also an insensitivity as to whether a Lyman opaque (first paper in Ref. [7]) or a Lyman transparent (second paper in Ref. [7]) case is considered.

In particular the very critical distribution of vibrational states in the molecules is very difficult to predict. It may, e.g., be dominated by wall effects, and certainly a collisional equilibrium as assumed here may not be established [9]. It may turn out to be necessary to treat vibrational transitions as an (in-elastic) relaxation process in computational models rather than within the frame of a collisional radiative model.

We conclude that due to the effects discussed here and the uncertainty involved the global parameter f_{fric} (not to mention its spatial distribution) must be regarded as poorly determined for divertor plasmas in the few eV range.

3. Momentum transport in the plasma free zone

In general, the neutral–neutral collisionality is too low (i.e., Knudsen numbers are typically larger than 0.1) to justify a fluid description of neutral particle momentum

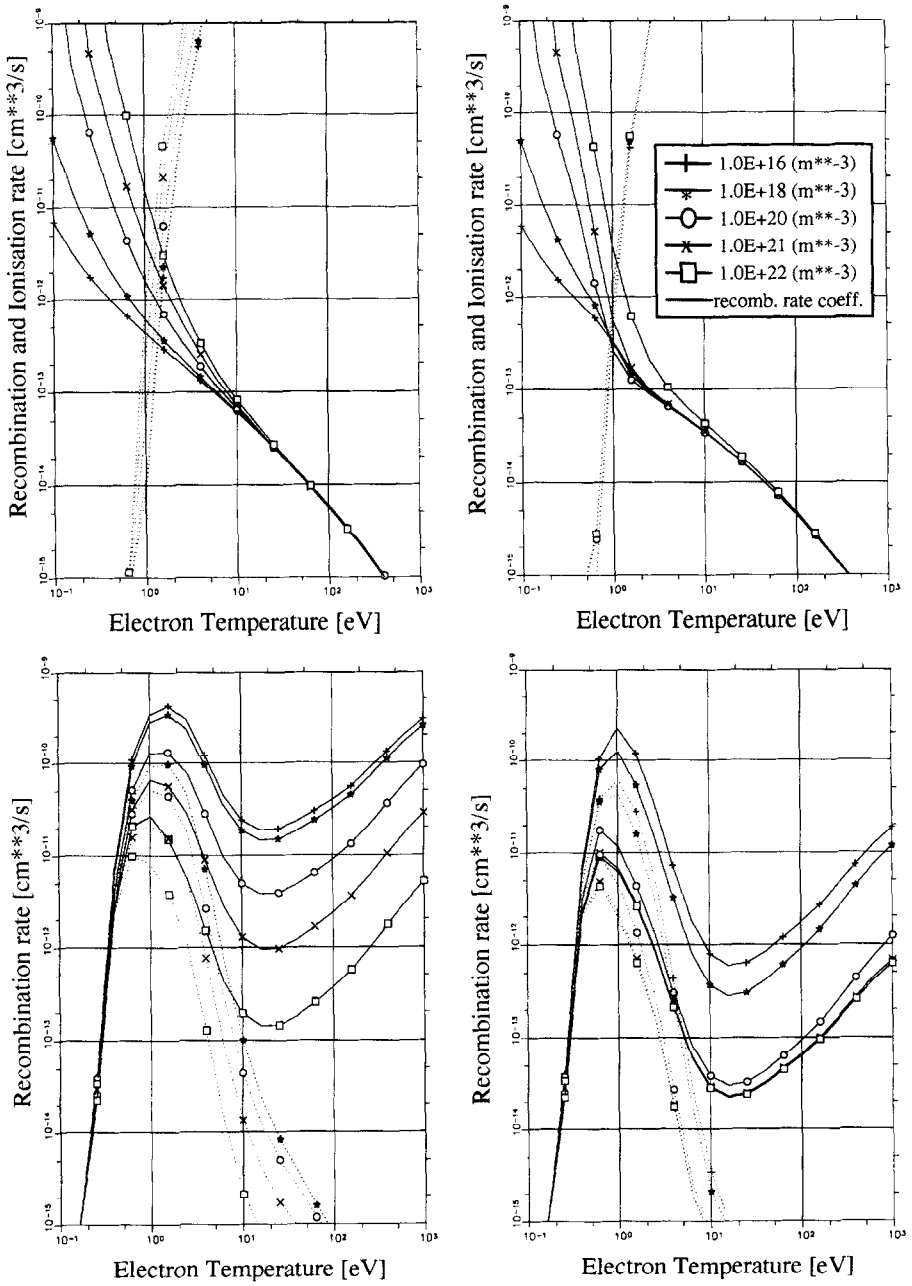

Fig. 1. Recombination rate coefficients due to radiative and three-body processes, $\langle \mathrm{rec} \rangle^{3+r}$ above, and due to H^- formation (dotted lines) and H_2^+ recombination (solid lines), $\langle \mathrm{rec} \rangle^{\mathrm{mol}}$, below, versus T_e, for 5 plasma densities, Lyman transparent conditions (left) and Lyman opaque conditions (right). Also indicated above: effective ionization rate coefficients (dotted lines).

transport. The full kinetic self-collision term for a gas mixture (species indices i, j) in the Boltzmann equation reads, using standard notations:

$$\frac{\partial f_i}{\partial t}_C = \sum_{j=1}^{s} \int_{-\infty}^{+\infty} \int_0^{4\pi} \left(f_i' f_j' - f_i f_j \right) c_{r_{ij}} \sigma_{ij} \, \mathrm{d}\Omega \mathrm{d}\vec{c}_{r_{ij}}. \qquad (1)$$

It is, except for highly idealized cases, even intractable for Monte Carlo integration although such procedures are well known. They are frequently applied to strongly idealized cases. If we wish to estimate the effects of self-collisions in the neutral gas in realistic configurations, we have to use 'model collision terms'.

We replace the collision integral by the BGK-expression:

$$\frac{\partial f_i}{\partial t}_{BGK} = \frac{(M_i - f_i)}{\tau_i} + \sum_{j \neq i} \frac{M_{ij} - f_i}{\tau_{ij}}. \quad (2)$$

M_j, M_{ij} are local drifting Maxwellians and τ_i, τ_{ij} are collisionality parameters (dimension: time).

The free parameters in the Maxwellians can be used to mimic features of the full Boltzmann integral.

The five parameters (density n_i, temperature T_i and drift velocity $\vec{u}_i$) in each self-collision Maxwellian M_i are fixed by the requirement to preserve the five collisional invariants 1, $\vec{c}$ and c^2 of the full Boltzmann integral.

For the 10 parameters arising in the mixed Maxwellians M_{ij}, M_{ji} for each combination (i, j), $i \neq j$, one has first conservation of particle number in each species (two constraints), secondly conservation of total momentum in the binary mixture (three relations) and finally conservation of total energy (one equation). The four final parameters can be obtained, for example, by comparing relaxation equations derived from the BGK-model term with corresponding relations derived with the full Boltzmann collision integral.

The equations for all the parameters in the Maxwellians (20 parameters for a binary mixture) depend on the choice of a force law for the particle interaction. We follow a practise common in the use of BGK models and choose collisionalities independent of velocity ('pseudo Maxwellian molecules'). This renders this set of equations particularly simple, and one finds for the cross-collision parameters ($\vec{u}_{ij}$ is the drift in M_{ij}) [10]:

$$\vec{u}_{ji} = \vec{u}_{ij} = \frac{m_i \vec{u}_i + m_j \vec{u}_j}{m_i + m_j}, \quad (3)$$

$$kT_{ij} = kT_i - \frac{2 m_i m_j}{(m_i + m_j)^2}\left[(kT_i - kT_j) - \frac{m_j}{6}(\vec{u}_i - \vec{u}_j)^2\right]. \quad (4)$$

Finally, the collision times τ_j and τ_{ij} are model parameters chosen to match either theoretical or experimental transport coefficients. Following, e.g., the Chapman Enskog procedure with the model collision terms, we can derive transport coefficients in terms of these collision times [11]. There is only one parameter for self collisions. We choose it to match experimental viscosity values $\eta_{H_2} = 1.25 \times 10^{-7}\, T_{H_2}^{0.75}$(Pa s) [12]. For atoms we first determine the self-diffusivity, D_H, using the experimental diffusion volume for atomic hydrogen $(\Sigma v)_H \approx 2$ (loc.cit.). Since for Maxwellian molecules the BGK terms preserve the Chapman Enskog relations between diffusivities and viscosities, we can then derive a viscosity for the atoms $\eta_H = 2.07 \times 10^{-7} T_H^{0.75}$ (Pa s).

The τ_{H,H_2} is chosen to match the mutual diffusivity $D_{H,H_2} = 8.91 \times 10^{19} T^{0.75}/n$ (m^2/s).

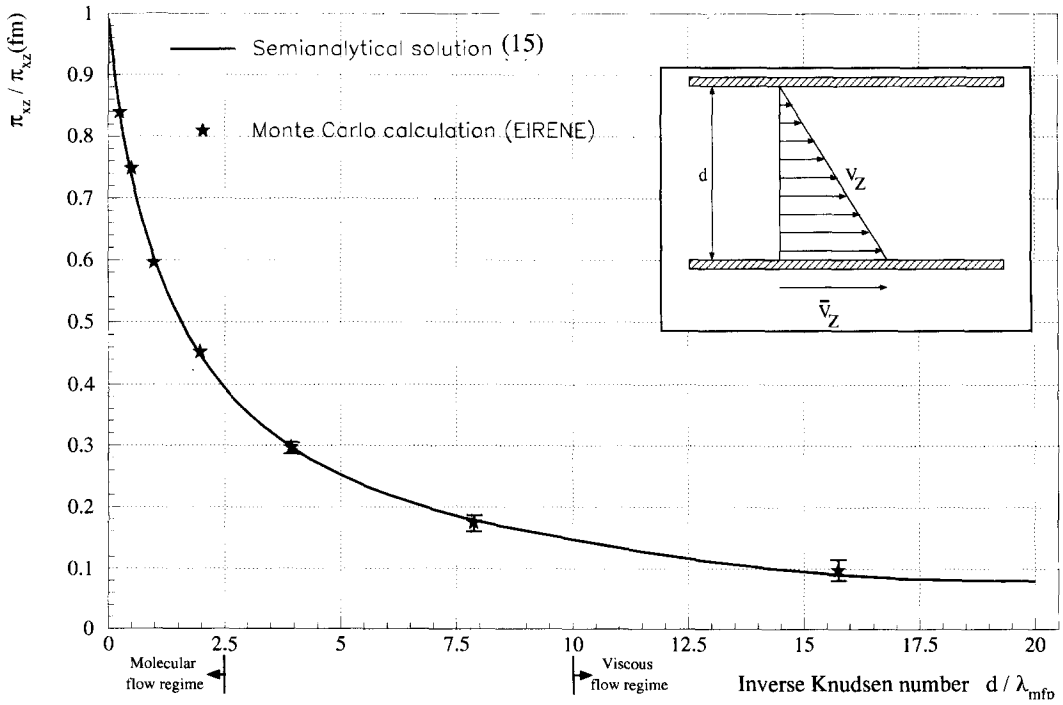

Fig. 2. Normalized stress tensor versus inverse Knudsen number for Couette flow problem. Comparison of analytical with Monte Carlo solution.

Finally the $\tau_{H_2,H}$ follows from the relation $\tau_{ij}n_j = \tau_{ji}n_i$ already used in deriving the above relations for the mixed moments.

3.1. Monte Carlo solution of non-linear BGK-equations

The non-linear equations for the parameters in the self-collision terms can be expressed in terms of appropriate functionals $\langle g_{k,i}, f_i \rangle$ of the distribution function f_i ($k = 1, \ldots, 5$ for the 5 collision invariants). Such functionals, for arbitrary moments g, but with f_i being a solution of linearized kinetic equations only, are provided by the Monte Carlo code EIRENE [13].

Therefore we use an iterative procedure ('successive linearization') to determine the parameters in the self collision terms. The cross-collision parameters can be evaluated after each iteration from these parameters by the algebraic Eqs. (3) and (4).

The BGK 'collision-integrals' arising during that iteration are special (and particularly simple) cases of the general linear elastic collision integrals already implemented in EIRENE [14].

The convergence of the iterative procedure is limited only by statistical noise in the linearized functionals $\langle g, f \rangle$, which, in principle, can be reduced to arbitrarily low levels by increasing the run-time of the code.

In order to check the algorithm, we have studied a plane Couette flow problem, for which semi-analytical and precise numerical solutions are available in the literature [15].

We consider a gas between two infinite parallel plates (distance d in x-direction), which move relative to each other in z-direction with velocity $V_{z,\mathrm{wall}}$. The Knudsen number of the flow is then given as $\lambda_{mfp}/d = \sqrt{2RT}/d \cdot \nu$ with collision frequency $\nu = 1/\tau = n\langle \sigma v \rangle$. The stress tensor element Π_{xz}, normalized to the free molecular flow

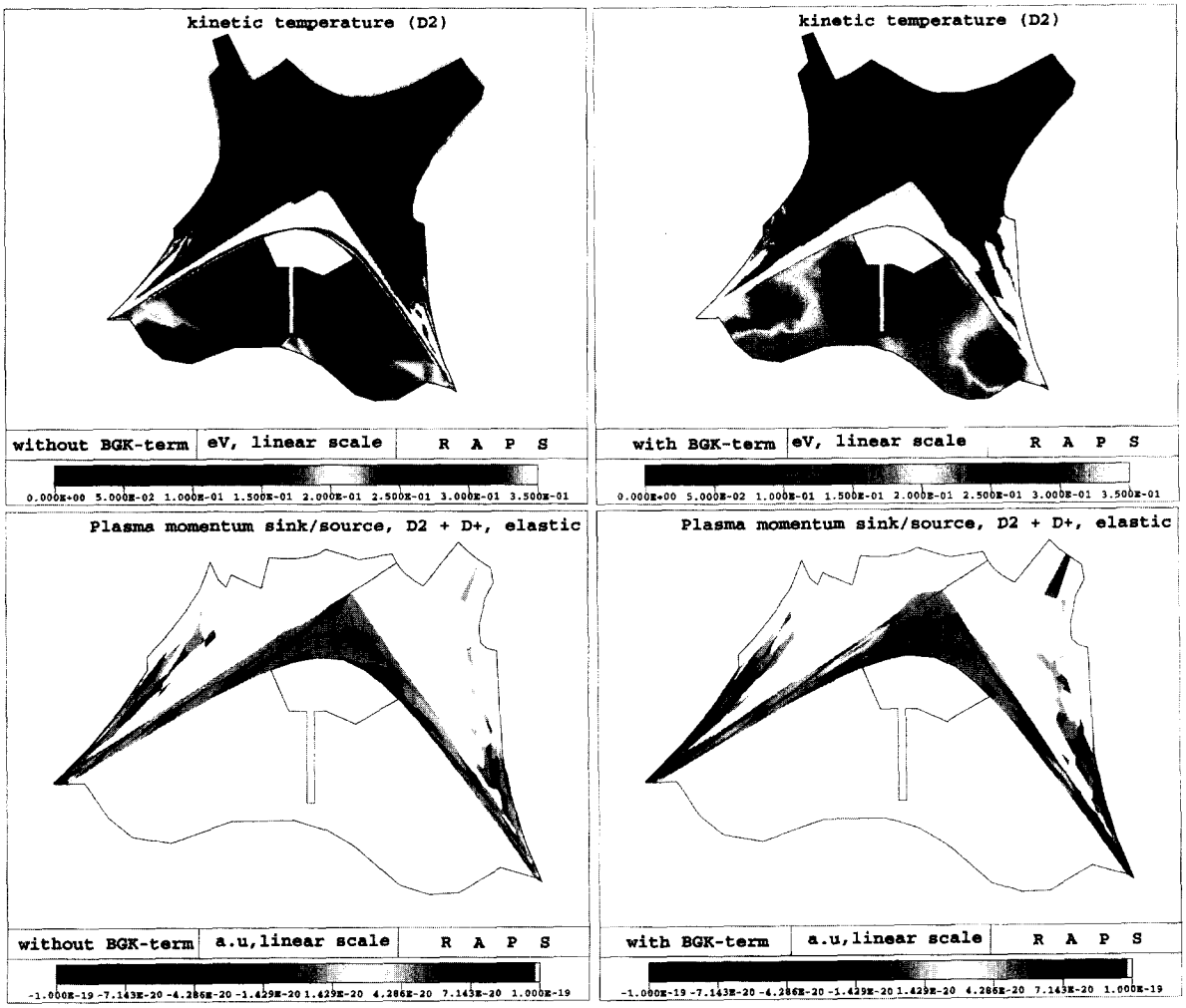

Fig. 3. Molecule temperature profile in divertor chamber (above), and plasma momentum sink due to elastic dipole H_2–H^+ interaction (below), without (left) and with (right) frictional effects in neutral gas mixture.

(fm) value $\Pi_{xz}^{\mathrm{fm}} = 1/4nm(8kT/\pi m)^{1/2}V_{z,\mathrm{wall}}$ is then a function of the Knudsen number alone. Perfect agreement is achieved by our Monte Carlo procedure (see Fig. 2). The number of iterations and Monte Carlo trajectories required to achieve a given error level increases strongly with decreasing Knudsen numbers. In our case with Kn = 0.05 (far in the viscous flow regime) 25 iterations with up to 250.000 trajectories each (about 24 h total run time each on IBM-RISK 6000 workstations) resulted in only 10% precision. For larger Knudsen numbers (of order 1) errors of the order of 1% and less are obtained after only 5–7 iterations (total cpu time: 30 min).

3.2. Application to the ITER divertor

A 1 dimensional computational assessment of momentum removal from divertors using the model described here is given in the accompanying paper [16]. We describe here results from a study of viscous effects in the divertor chamber under less idealized conditions. . It was obtained from B2-EIRENE [1] code simulations of a low (non-radiated) power (25 MW) medium density ($n = 7.5 \times 10^{19}$ (m^{-3})) SOL, with pumping in the bottom of the divertor such that flux amplification factors of order 50 result. The inner target is partially detached then, the outer (pumped) target is still in high recycling conditions. The orthogonal grid for B2-EIRENE was originally obtained with the Sonnet code [2], but for the applications here replaced by an unstructured mesh of triangles extending also in the vacuum region.

Only intrinsic neutral particle sources, i.e., no gas puffs, etc., are considered: three body volume recombination (not including the enhancement factors discussed above), is 1.25×10^{23} (1/s) and divertor target recycling is 3×10^{24} (1/s).

This choice of model parameters and configuration results in Knudsen numbers of the order of unity for molecules (and larger for atoms) in the divertor chambers, and leads to converged non-linear results (for a noise level as achieved by the 7000 neutral trajectories in each iteration) after five iterations.

A comparison of results from a case with and without the non-linear BGK collision terms (see Fig. 3a, b for the molecule temperatures in the divertor) shows, as expected, an incomplete relaxation of temperatures between molecules and atoms near the plasma legs.

The total parallel momentum sink in the SOL due to charge exchange friction between atoms and ions (related to f_{fric} in the terminology of Section 2) increases by about 20%. Note that atoms are, in general, much less effected by viscous effects in the gas, than molecules. Rather subtle velocity space effects seem to play a role here, probably caused by a deeper penetration and dissociation of the now hotter molecules (Fig. 3). By a similar amount, however, the momentum sink in the plasma due to elastic dipole H_2–H^+ collisions (same order of magnitude as CX-terms in this case), is reduced. This latter observation can more easily be understood from viscosity effects in the plasma free region, e.g., as 'non-perfect momentum accommodation' for neutral molecules at the interface between plasma and plasma free region. Such effects have already been discussed on the basis of analytical considerations under simplifying assumptions [17].

In general, momentum removal from the divertor plasma is determined, firstly, by the efficiency for the neutral gas to pick up momentum in the plasma, and secondly by its efficiency to transport that momentum to the side walls. Certainly, viscous effects in the neutral gas reduce the second of these efficiencies, and more strongly for molecules than for more energetic atoms. However, the above mentioned results indicate that under certain conditions this can be compensated by an increase in the first efficiency, here due to enhanced momentum accommodation for atoms in the plasma fan.

The total elastic momentum exchange in the toroidal direction due to self-collisions (strictly zero in the BGK model) was converged to 0.05% of the frictional loss in the plasma, both for atoms and for molecules. A transfer of toroidal momentum from atoms to molecules of about 1% of the CX frictional term persists, and of similar magnitude (with opposite sign, i.e., a sink) from molecules to atoms. Total momentum between molecules and atoms is conserved down to a level of 0.1% of the CX friction term.

Fluxes to the albedo surfaces (for pumping) at the bottom of the configuration have not been altered in a statistically significant way (i.e., if at all, then by less than 5%). Hence Knudsen numbers of the order one, as established here, appear not to be sufficient to establish any significant increased flow towards pumps. The cases considered here may even happen to be in a regime, in which, under other configurational conditions, the 'Knudsen-paradox in Poiseuille flow' of decreased flow rate despite increased collisionality is observed experimentally, and well explained by BGK collision models such as the one used here [15].

4. Conclusions and outlook

The role of molecules in plasma recombination has been reconsidered, and was shown to be significant but probably less dramatic than simple estimates would indicate. However, the friction between neutral particles and the divertor plasma may still be affected by such processes. The momentum transfer from the plasma to the neutral particles and hence plasma conditions near the divertor target may even be affected strongly.

The transport of plasma momentum to the walls via the neutral particles is furthermore determined by the self-collisionality (Knudsen number) in the divertor and requires revision of current neutral gas transport models.

A procedure to extend linear Monte Carlo models from the 'molecular flow' regime into the 'transition flow'

region based on BGK-type model collision terms has been developed and tested. It is applicable in otherwise arbitrarily complex configurations, background plasma conditions and boundary conditions. The current numerical performance of the algorithm ceases to be acceptable in the viscous flow regime with Knudsen numbers less than 0.1.

For a Couette flow problem the accuracy of the algorithm could be demonstrated by comparison with analytical solutions. We conclude that the code should be able to treat general transition flow regime problems (Poiseuille flow, shock structure) under much less restrictive conditions than hitherto present in numerical procedures.

The free collisionality parameters in the model are chosen to match empirical viscosity and diffusivities in atomic and molecular hydrogenic gases. We have applied the model to an ITER sized divertor configuration and plasma.

The viscosity in the neutral gas seems to effect momentum removal by atoms and molecules differently, due to velocity space effects. It has, probably, to be investigated on a case to case basis.

The atom and molecule temperatures in the divertor chamber relax towards each other, but, nevertheless, remain significantly distinct. Hence the validity of fluid descriptions assuming perfect thermalization appears to be questionable under such conditions.

The additional iterations required to include the neutral–neutral collisions in the B2-EIRENE code system further increase the computational complexity. We suggest that it is useful first to parameterize momentum accommodation coefficients (versus Knudsen number) for the computational boundaries separating the divertor plasma from the 'vacuum' (plasma free) region by the procedure outlined here and then to simulate the plasma region with only these boundary conditions using e.g., the B2-EIRENE code. This should result in more realistic treatment of frictional effects in divertors close to and after detachment.

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