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NEUTRAL PARTICLE KINETICS IN FUSION DEVICES

By

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ABSTRACT

The theory of neutral particle kinetics treats the transport of mass, momentum, and energy in a plasma due to neutral particles which themselves are unaffected by magnetic fields. This transport affects the global power and particle balances in fusion devices, as well as profile control and plasma confinement quality, particle and energy fluxes onto device components, performance of pumping systems, and the design of diagnostics and the interpretation of their measurements. This paper reviews the development of analytic, numerical, and Monte Carlo methods of solving the time-independent Boltzmann equation describing neutral kinetics. These models for neutral particle behavior typically use adaptations of techniques developed originally for computing neutron transport, due to the analogy between the two phenomena, where charge-exchange corresponds to scattering and ionization to absorption. Progress in the field depends on developing multidimensional analytic methods, and obtaining experimental data for the physical processes of wall reflection, the neutral/plasma interaction, and for processes in fusion devices which are directly related to neutral transport, such as H_α emission rates, plenum pressures, and charge-exchange emission spectra.

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1. INTRODUCTION

Immediately after the problem of building a controlled thermonuclear reactor was formulated, it was realized that neutrals constitute an important component at the periphery of the fusion device owing to the significant wall recombination of the plasma which is lost from the discharge and must be returned back as neutrals in the steady state (1). The original outline of a basic model for neutral transport in confined plasmas is given by Sacharov (2). The atoms may charge-exchange, creating a new atom with a new velocity that continues to either charge-exchange, be ionized, or strike the wall. Through charge exchange or wall reflections, new generations of atoms are formed and move through the plasma interior. The molecules dissociate upon entering the plasma creating atoms and ions with approximately 5 eV of energy. The resultant ions start their own cascades. A graphical depiction of different channels for neutral kinetics is shown in Fig. 1.

The theory of neutral particle kinetics treats the transport of mass, momentum, and energy in a plasma due to neutral atoms or molecules which are unaffected by magnetic fields. Global plasma phenomena affected by this transport include the following aspects of fusion research:

Global power and particle balance. Neutral particles refuel the plasma as they are ionized by plasma particles, adding also to the plasma's momentum and energy. The need for particle exhaust in fusion devices stems from requirements for impurity control, density control, and fusion product (helium) removal. Thus, it is important to study the mechanism of plasma refueling and exhaust. This mechanism may also include external sources or sinks of neutrals, such as pellet or neutral beam injection and gas puffing, as well as the recycling of neutral atoms and molecules formed as plasma ions strike device walls. The processes of charge-exchange and ionization alter the plasma momentum and energy. Plasma electrons lose energy as they excite and ionize neutral particles and dissociate molecules.

Profile control and plasma confinement quality. The distribution of the particle and energy sources and sinks strongly influences plasma density and temperature profiles, which are important for plasma equilibrium and stability properties. Given a certain capability to control these profiles, the spatial distribution of sources may be an important mechanism in attaining the improved confinement regimes observed during divertor operation in the ASDEX, PDX, and Doublet tokamaks (the H-mode); pellet injection experiments in

ALCATOR-C; and impurity feeding on ISX (the Z-mode).

Particle and energy fluxes to device walls. Neutral particles transmit energy to the confinement device's walls through radiation and collisions with them.

Erosion of device walls due to sputtering. Sputtering by charge-exchange neutrals may be a major source of impurities in the plasma, and is an important factor in the design of machine components exposed to high heat and particle fluxes. Although a limiter can protect the first wall from bombardment by plasma ions, it cannot shield the first wall from being bombarded by energetic neutrals generated in the inner core as a result of recombination and charge-exchange with neutral beams. However, this process differs from sputtering by plasma ions since neutrals are not accelerated by the electrostatic sheath formed in front of solid surfaces. Under certain conditions the boundary layer of a tokamak could be made impermeable to incoming high energy neutrals in order to avoid significant damage and erosion of the wall's structures. On the other hand, neutrals with low energy are quite convenient energy carriers (as convenient as photons), since they do not produce sputtering. Neutrals distribute the energy homogeneously over the inner surface of the plasma chamber.

Level of tritium contamination in device walls. The charge-exchange flux is a major mechanism in tritium contamination of the first wall in a D+T machine. For example, it is necessary to know this flux in order to schedule tritium discharges in TFTR and JET.

Performance of pumping systems. Future reactors will have to be pumped to remove impurities, in particular helium, so as to sustain long-pulse operation. Ideally, the impurities would be preferentially removed from the reactor, leaving relatively more of the tritium fuel in the system. The physics of how to do this is, at this moment, highly speculative. Among the unknowns are the relative confinement in the main discharge of hydrogen versus helium, the relative intensity of their recycling, and the difference between the two species in the pumping efficiency of proposed pump designs.

Interpretation and design of diagnostics. Knowledge of neutral transport behavior is also necessary for the design and analysis of such widely used experimental diagnostics as neutral particle emission analyzers, H_α -emission detectors, and pressure gauges. The neutral density also affects the relative populations of ionized states of impurities, such as oxygen and carbon, via

charge-exchange recombination, and hence must be known when interpreting spectroscopic measurements of lines from these elements.

The following physical processes affect neutral kinetics.

Neutral-plasma interactions. A catalogue of reactions for hydrogenic atoms and molecules, and helium atoms is given in Table 1. Recent reviews of existing atomic wall reflection experimental and theoretical data can be found in Refs. 3-11.

While much of the basic relevant atomic physics can be described in theory, there remain outstanding problems whose solutions are important in our modeling. One of these is that in order to compute the rate of H_α emission, we must be able to determine the excitation states of hydrogen in systems where the atom will be not in thermal equilibrium with the ambient plasma. For example, an atom in the throat of a narrow pump limiter may cross the throat in 10^{-7} sec, which is roughly the same time scale as the excitation and de-excitation processes. The excited state may also be changed while striking the wall. Another completely unknown is the influence of the vibrational states of molecular hydrogen on the reaction rates. This process may absorb relatively large amounts of energy in a divertor. There are also large gaps in the measured data for reaction rates, and where the data exist, there are uncertainties in them. One difficulty is that the range of temperatures found in controlled fusion devices is large, from 1 to 10^4 eV, and we may need the reaction rates over the whole range in particular calculations.

Neutral-neutral and neutral-ion elastic scattering processes. When the ambient neutral density rises above 10^{14} cm^{-3} , elastic scattering becomes important. Presently, there are little data on total cross section for H^0 and D^0 onto anything at energies above 2 eV and below 300 eV. Some data for 25 to 1800 eV D^0 and He^0 onto He, Ne, Ar, and Kr that were measured utilizing PLT as a neutral particle source and the Low Energy Neutral Spectrometer as a detector appear in Ref. 12. However, in pump ducts where we may find high neutral pressures, the atomic energies are below 25 eV, for which there are no data.

The process of wall reflection. The reflection probability, distributions of reflected energy, reflected angle, and physical sputtering yield, are all functions of the incident particle species, energy, and incident polar angle, as well as target composition, surface roughness, and surface contamination.

Most existing reflection data are for well-characterized wall materials

with clean and smooth surfaces. Relatively few projectile/target pair have been treated, with incident energies typically above 100 eV. This restriction in energy is due both to the difficulty in generating neutral beams of energy less than 50 eV, and the theoretical problem of treating the multibody interactions which become important at energies of a few eV (13). A key question is how different from the ideal case is wall reflection off the rough and dirty walls actually found in fusion devices.

The process of desorption of sticking particles also affects the source rate for neutral particles. This process depends on the depth distribution of particles absorbed in the wall, the impinging particle flux, wall temperature, and aspects of the wall structure.

The plasma sheath. The properties of the sheath created when the plasma strikes a wall determine the distribution in energies of the neutral particles produced at a neutralizer plate.

Molecular processes. The problem of transport of heavier neutral molecules is largely unexplored by experimentalists. For example, methane forms on a carbon surface when exposed to a hydrogen plasma, and methane and water are produced in stainless steel when it is struck by carbon and oxygen impurities. In order to model neutral molecular transport, it is necessary to have data on the production rate and the type of molecular impurities produced at the walls, and data describing the molecular/plasma interaction.

2. ANALYTICAL METHODS

We assume that the Boltzmann equation describing the neutral particle distribution $f(\underline{x}, \underline{y})$ over position, $\underline{x}$, and velocity, $\underline{y}$, space is time independent

$$\underline{y} \cdot \text{grad } f(\underline{x}, \underline{y}) = C(f)(\underline{x}, \underline{y}) , \quad (1)$$

where $C(f)$ is the neutral/plasma collision integral.

Analytic solutions of the kinetic equation are described in this section, and numerical and Monte Carlo solutions are discussed in Secs. 3 and 4.

Solving Eq. (1) in three dimensions is a formidable task and methods to do so were found only recently. We describe in this section analytical methods of solving Eq. (1) applicable only for the one-dimensional studies.

Analytical methods to study the neutral dynamics are useful for a number

of reasons. One of them is that the description of the neutral gas-plasma interactions is very strongly dependent on the data from the atomic, molecular, and plasma-wall interactions studies. Though quite extensive information has been accumulated in these fields, the work is far from being complete and a number of coefficients required for solution of the problem are either uncertain or unknown. So it is of interest to work out analytical solutions which contain most of the essential features of the problem, and which allow for future incorporation of new information as soon as it becomes available.

Another reason is that the information on the neutral component is usually used in one-dimensional plasma transport codes. These codes can be significantly simplified not by including neutrals explicitly, but by accounting for them through the boundary conditions, which would follow from a separate study of the edge region where neutral effects are significant. The easiest way to do this is with one-dimensional analytic solutions, when possible.

Two- and three-dimensional calculations for neutrals require two- and three-dimensional plasma profiles. The latter are not always very well known and often imply additional assumptions.

A final advantage of analytical solutions over numerical algorithms is that parametric dependencies are more easily observed from them. Numerical algorithms used on computers must be verified before one can have complete confidence in them, and analytical solutions available for simplified situations provide a useful tool for this purpose. Thus, they are important complements to numerical codes and may be used for either model calculations or as a method to verify the latter under the same conditions.

A. One Species Models

Analytical methods were employed for studies of neutral kinetics early in the history of fusion research. Sacharov (2) gave the first analytic solution for neutral transport (Fig. 2), adopting existing solutions for neutron transport. He pointed out the analogy between the neutral and neutron kinetics, and adopted the solution for the latter known to him through fission reactor studies. The analogy assumes that the neutron absorption is equivalent to the ionization of neutrals, and the scattering of neutrons corresponds to the charge-exchange processes for neutrals. Though this

analogy is not complete (we defer the quantitative discussion of this statement to later in this paper), it should be emphasized that this observation has been extremely fruitful for the subsequent development of the subject, and has been used by many authors in choosing their methods of mathematical analysis.

Using the assumption of the complete analogy between these physical processes, Sacharov estimated that the albedo of the plasma to the hot neutrals varies as the square root of the ratio of the probabilities of the charge exchange to ionization (2). He also was the first one to realize that one component of hydrogen neutrals attains the energy of the plasma particles by multiple charge-exchange, and penetrates much deeper into the plasma than the component attenuated directly by electron impact ionization. His argument was that though the difference in average velocities of these two components is very large (the fast neutrals have the mean velocity of the plasma particles and the slow ones have the temperature of surrounding walls), the time between collisions with plasma particles is almost the same for both species. It implies a significant difference in their mean-free paths. The heat flux required to support a structure with a temperature gap between the plasma and the walls of the order of ten electron volts has been estimated as 50 W/cm^2 , which is rather close to the value conjectured for INTOR.

His work has been extended by his associates Zubarev and Klimov (14). Their model was based on the Sacharov idea that as the density and the size of plasmas increase approaching the reactor regime, the plasma gets impermeable to neutrals. Thus, the neutrals are confined to a narrow surface layer. The easiest way to formalize this criterion is to determine the Knudsen number, $K = \lambda/L$, where λ is the mean-free path length of the thermal neutral and L is the characteristic length of the problem. If $K \ll 1$, even in a narrow layer, it is possible to consider the problem as one-dimensional, i.e., dependent only on the distance x from the boundary.

Zubarev and Klimov assumed that the distribution function of the charge-exchange neutrals has the same parametric dependence on the velocity as the ion distribution function. (The validity of this assumption will be discussed later in this section.) It yields the following kinetic equation for fast neutrals:

$$u \partial f_n / \partial x + f_n = (B/2) n_n, \quad (2)$$

where f_n and n_n are the distribution function, averaged over the angle in the velocity space, and density of fast neutrals, respectively; β is the ratio of the charge-exchange rate to the total reaction rate for a neutral; and μ is the cosine of the angle between the neutral velocity and the normal to the wall. This equation is completely analogous to the equation employed in the neutron transport theory. They quoted a solution of Eq. (2) from the work of Romanov obtained by the Wiener-Hopf method. The results of their calculations are shown in Fig. 3. This method of solution corresponds to using the step function $f_i(u) = 1/2$ for $-1 < u < 1$, and $f_i(u) = 0$ for $u < -1$ and $u > 1$ as the ion distribution function.

The solution for the neutral profiles has been used to formulate boundary conditions for the plasma density and temperature profiles. The absolute value of the incoming neutral's density has been estimated to be of the order $10^{11}/\text{cm}^3$ at the wall for an energy flow of 6 W/cm^2 , a particle flow $4 \times 10^{17}/\text{cm}^2\text{sec}^{-1}$ and the average plasma density $10^{14}/\text{cm}^3$.

The first application of the neutral component for the purpose of the plasma diagnostics was made on the device "Alpha" in the Lofte Institute by Afrosimov *et al.* (15). The energy distribution of the outgoing fast neutrals was measured. In connection with these measurements the question arose as to the extent to which this distribution reflects the energy distribution of the plasma ions. The theoretical analysis of this question has been performed in (16). Their basic argument was that the distribution function is an integral function of the neutral density and therefore only slightly dependent of the fine details of the neutral density profile [see Eqs. (13a-b)]. For the case of homogeneous plasma density profile, they obtained the crude solution for the neutral density, assuming the form $1/2 [\delta(v-v_{th}) + \delta(v+v_{th})]$ for the ion distribution function. The solution has been obtained as a simple algebraic expression. The slow component of the neutrals followed from it instead of being assumed ad hoc. The expression for the flux of the outgoing neutrals taken at the wall was derived, and three components were shown to exist: the singly charge-exchanged, multiply charge-exchanged, and unattenuated neutrals. The albedo of the plasma for neutral atoms was given as:

$$A = 1 - \{1 + v/v_+\} \sqrt{1-\beta}/v/v_+ + v/v_+ \sqrt{1-\beta} \quad , \quad (3)$$

which, under the condition that the plasma temperature equals the neutral injection energy, $v=v_+$, coincides with the result of Ref. 2.

As fusion research developed towards longer pulses and confinement times, it became clear that the plasma in the fusion device could hardly be isolated from the wall by a vacuum region. In 1960 quite a different system was considered by Alfvén and Smars (17). Instead of having the plasma surrounded by vacuum, it was suggested that one should start up a discharge with the vessel filled with gas at atmospheric pressure, and fully ionize and heat only a small volume of the gas in the center of the vessel using a magnetic field for confinement of the hot core. The hot plasma would thus be separated from the walls of its container by a high density, weakly ionized gas. The subsequent experiments performed to test this idea have shown that, depending on the initial phase of the high pressure discharge, a low pressure pinch surrounded by a cool, high density gas region, can be attained on the short time scale of around 5 μ sec, limited by the development of plasma instabilities. However, on this short time scale, impurities from the walls were effectively prevented from reaching the hot region, thereby leading to an extremely clean plasma.

This idea was suggested before limiters were used to define the plasma edge and to prevent direct contact between the plasma and the vacuum chamber walls (18). Use of limiters was one of the key factors leading to cleaner plasmas on much longer time scales.

Lehnert (19,20) analyzed the equilibrium conditions (particle, momentum, and energy balances) of the then existing and future reactor experiments, and came to the conclusion that the main question is whether or not the penetration of the neutral gas can be made consistent with the transport properties of the plasma. The result from this self-consistent approach was the so-called diffusion approximation for neutral dynamics. Using fluid equations, the neutral density profile was described by the ordinary diffusion equation with coefficients dependent on the plasma profiles.

The essential features of this model are as follows. In a steady state, using a one-dimensional slab approximation, the outward plasma flux, nv , was assumed to be balanced by an inward neutral flux, $n_n v_n$, so that the particle balance reads

$$d(n_n v_n)/dx = -d(nv)/dx = -nn_s \quad (4)$$

Here S is the effective electron impact ionization rate. The plasma pressure, nT , in the boundary layer was assumed to be balanced by the magnetic field, B

$$2d(nT)/dx = -B^2v/\Sigma \quad (5)$$

while the pressure of the neutral gas was balanced by friction with ions predominantly through charge-exchange collision, i.e.,

$$d(n_n T_n)/dx = -mCn_n(v_n - v) \quad (6)$$

Here n , T , v and n_n , T_n , v_n are plasma and neutral densities, temperatures, and fluid velocities, respectively; C is the friction force coefficient owing to charge exchange; B is the magnetic field; and Σ is the plasma conductivity.

The following further assumptions were made. Instead of using the energy balance, temperatures of ions and neutrals were assumed to be equal and independent of x . The plasma density was assumed to be much larger than the neutral density throughout the layer, and only the $v \times B$ force was included in Ohm's law. Integrating Eq. (4) over the boundary layer and substituting into Eq. (6), we get

$$d^2 n_n / dx^2 = n_n / \delta^2 \quad (7)$$

Under the assumption of constant plasma density and temperature, the diffusion coefficient is then $D = v_{th} \lambda_{ch-ex} / 2$, and the penetration depth of the incoming neutrals is $\delta = \sqrt{\lambda_{ion} \lambda_{ch-ex} / 2}$. The physical reason for this is that if the probability for neutral particles to charge exchange is much greater than the probability to ionize the process of penetration becomes a random walk with the elementary step size equal to the mean-free path length for charge exchange. However, the fluid approach becomes invalid when plasma parameters change over the mean-free path lengths of neutrals.

Another important point taken up by Lehnert is the classification of different plasma density regimes with respect to neutral gas penetration. This classification is through the average ion density, n , and the characteristic macroscopic dimension, L . It is based upon the estimate [see Eq. (7)] that the product $nL \approx 10^{15} \text{ cm}^{-2}$ is almost independent of the average ion density. This estimate led to the classification of tokamaks as permeable

or impermeable depending on whether the fast charge-exchange neutrals penetrate the whole of the plasma or are limited to a narrow boundary layer.

At that time most machines were permeable, but it was clear that a full-scale reactor would operate in an impermeable regime. Several effects play an important role. The penetration of neutrals into the interior is determined by charge exchange and ionization. The probability of fast neutrals, produced by charge exchanges in the hotter regions, to reach the wall is a function of their energy and the line-integrated density they have to traverse. Thus the impurity productive via charge exchange depends on the neutral gas density and temperature at the periphery and the plasma temperature profile (21), and is also a steep function of the line-integrated density from the walls. The sputtering efficiency of neutrals increases drastically with their energy. The outgoing flux of energetic neutrals, deleterious due to sputtering of impurities, is strongly attenuated if the impermeability criterion is fulfilled. TFTR, JET, and JT-60 are the first generation of devices approaching the impermeable regime.

ASDEX-Upgrade, a tokamak experiment with a reactor compatible poloidal divertor, was designed to guarantee a value of nL required for impermeability. It is now under construction at Max-Planck-Institute für Plasmaphysik in Garching. The extensive computer runs made during the design phase confirmed the picture outlined above, and refined the criterion for the boundary zone width to be $\int n dr > 2 \times 10^{15} \text{ cm}^{-2}$, where the integral is taken between the wall and the isotherm of $T_{\text{plasma}} = 300 \text{ eV}$ (22).

An analytic solution for the neutral density profile has been derived by Rehker and Wobig in a paper (23) whose main results were obtained numerically, and which were compared with an analytical solution under assumptions of constant plasma density and temperature. Although derived independently, their analytic solution seems to coincide with the solution obtained in Ref. 16. It has been shown that the numerical results for the neutral density are rather close to the analytical, though some special forms for the ion distribution are used to obtain them.

Another important point taken up by them is the influence of the reflection mechanism of outgoing neutrals at the wall on the neutral dynamics. What is required is an algorithm for choosing the outgoing energy and angles of emission for an incident particle with a given incident energy and angle to the normal. It should be emphasized here that such algorithms

are not exact at present. In the analytical approach the algorithm is introduced through the boundary conditions taken in the most general form as:

$$f_+ = f_+^0(v) + R_s f_-(0, -v) + R_d f_d(v) \int v f_d^3 f. \quad (8)$$

Here R_s and R_d are the coefficients of specular and diffuse reflection, and $f_+^0(v)$ describes neutrals emitted from the wall by plasma recycling, thermal desorption, etc. This distribution $f_+^0(v)$ consists of the flux of Franck-Condon and cold neutrals owing to the recombination of plasma at the wall and subsequent backscattering as neutrals atoms or molecules. The distribution $f_d(v)$ describes the very important physical process of the energy degradation upon reflection and is normalized by $\int v f_d^3 v$.

The flux of the specularly reflected neutrals is a very sensitive function of energy. The low energy neutrals are reflected in all directions with the original energy. The hot population impinges more perpendicular to the wall. Since the energy reflection coefficient decreases drastically with increasing energy, this population is lost upon reflection. Moreover, due to the inhomogeneous structure of the surface and additional reflections caused by it, neutrals are scattered in all directions with much lower energies. So the case considered by several authors of ideal specular reflection $R_s = 1$ and $R_d = 0$ is unrealistic. Note too that if the wall is covered with absorbed neutrals, the flux of the reflected neutrals may be larger than the flux of the outgoing neutrals ($R_d > 1$).

Introducing reflection at the wall modified the computed density profile of neutrals by a factor of 2-4 (23). This result emphasized the importance of surface physics data for this problem and indicated that the full solution in all its complexity requires sophisticated numerical methods. These boundary conditions make this problem similar to the albedo problem in astrophysics research considered by Chandrasekhar (24).

The collision integral was simplified as described in Ref. 23 and reduced to a tractable form which became widely employed in the literature. Therefore, we briefly describe the derivation of the formulation given in Ref. 21.

Provided we consider plasma temperatures less than approximately 1 keV, we can neglect ionization by impact with plasma ions, with the result that the contribution to the collision term from ionization becomes the following loss

term:

$$\int |v - v_e| \sigma_e f_e(v_e) d^3 v_e f_n(v) , \quad (9)$$

where $f_e(v_e)$ is the electron distribution function, σ_e is the cross section for ionization by electrons, and $f_n(v)$ is the distribution function of neutral particles. Clearly, the neutral velocity is much less than the electron velocity, and taking a Maxwellian velocity distribution for electrons with constant temperature and a density distribution $N_e(x)$, we get for expression (9)

$$- \langle \sigma_e v \rangle f_n(v) N_e(x) , \quad (9')$$

where $S = \langle \sigma_e v \rangle = \int v_e \sigma_e(v_e) f_e(v_e) d^3 v_e$ is independent of the velocity of the neutral particles.

The charge-exchange process on the ion distribution function $f_i(v')$ takes the form

$$\int |v - v'| \sigma_{ch-ex} [f_n(v') f_i(v) - f_n(v) f_i(v')] d^3 v' , \quad (10)$$

where σ_{ch-ex} is the charge-exchange cross section. To simplify the integral for charge-exchange collisions, we may assume that $|v - v'| \sigma_{ch-ex}$ is a slowly varying function of the relative velocity and replace it by a constant C , so that the charge-exchange term (10) takes the form

$$N(x) C [f_i(v) \int f_n(v) d^3 v - f_n(v)] , \quad (10')$$

where it has been assumed that $N_e \approx N_i = N(x)$ and the ion distribution is represented by a local function $f_i(x, v) = N(x) f_i(v)$.

Recombination is taken into account by including

$$f_i(v) \int v_e \sigma_{rec}(v_e) f_e(v_e) d^3 v_e , \quad (11)$$

where σ_{rec} is the recombination cross section. The kinetic equation can now be written as

$$v_x \partial f_n / \partial x + (\langle v \sigma_{ch-ex} \rangle + \langle v \sigma_e \rangle) N f_n = v \sigma_{ch-ex} N f_i \int f_n(v) dv + \langle v \sigma_{rec} \rangle N f_i. \quad (12)$$

Reparameterizing by the neutral optical depth

$$y = \int N(x) (\langle v \sigma_{ch-ex} \rangle + \langle v \sigma_e \rangle) / v_{Ti} dx, \quad ,$$

where v_{Ti} is the ion thermal velocity, and integrating over velocities v_y and v_z , we obtain from Eq. (12)

$$u \partial f_n / \partial y + f_n = \beta f_i \int f_n dv + \chi f_i N, \quad (12')$$

where $u = v_x / v_{Ti}$ is the dimensionless neutral velocity, β is defined as $\sigma_{ch-ex} v / (\langle \sigma_{ch-ex} v \rangle + \langle \sigma_e v \rangle)$, and χ as $\langle \sigma_{rec} v \rangle / (\langle \sigma_{ch-ex} v \rangle + \langle \sigma_e v \rangle)$.

It is easy to obtain the formal solution of Eq. (12') considering the right-hand side of Eq. (12') as a given source function. It yields the following expressions for the incoming and the outgoing neutral distributions

$$f_+(y, u) = f_+(0, u) \exp[-(y/u)] + f_i(u)/u \int [\beta n_n(y') + \chi N(y')] \exp[(y'-y)/u] dy', u > 0 \quad (13a)$$

and

$$f_-(y, u) = -f_i(u)/u \int [\beta n_n(y') + \chi N(y')] \exp[(y'-y)/u] dy', u < 0. \quad (13b)$$

Integrating Eqs. (13) over velocity spaced yields an integral equation for the neutral density

$$n_n(y) = n_0(y) + \int K(y' - y) n_n(y') dy', \quad (14)$$

where $n_0(y)$ and the kernel $K(y)$ are determined by the boundary conditions and the form of the ion distribution, respectively.

It is convenient to solve this integral equation numerically by iterations (see Sec. 3). In their simplest form (without accounting for the effect of the temperature gradients and the recombination), it yields

$$n_0(y) = n_0(0) \exp[-\int v_i / v_+ dy], \quad (15)$$

$$K(y) = \beta \int f_i(u) [\exp(-|y|/u)] / u du, \quad (16)$$

where $n_0(0)$ is the density of neutrals at the wall and v_+ is their injection velocity.

The expressions (13a) and (13b) when multiplied by the velocity give the atomic flux per unit plasma surface and per unit solid angle in a direction perpendicular to the plasma surface. They are very useful for diagnostic applications and give the spectra of neutrals ejected by the plasma.

Assuming that ions and neutrals have the same isotropic distribution, for example $f_{i,n} = \delta(u-1)/4\pi$, which allows us to integrate over the angle in the velocity space, we get an equation identical to the kinetic equation for neutrons [Eq. (2)]. We conclude that the possibility of using the sophisticated neutron transport codes to solve the neutral transport problem requires the assumption that the neutral distribution is isotropic as a source and remains isotropic under charge-exchange collisions. This assumption, which will be discussed later in more detail, represents a rather stringent constraint.

The next step in the development of analytical methods was undertaken by Connor in (25). The method of singular eigenfunctions, highly developed for the neutron transport problems, and summarized by Aamont and Case (26), was modified for the problem of penetration of neutrals into the dense plasma using a realistic Maxwellian ion distribution. This technique is intimately related to the Wiener-Hopf method, used by (14). In the simplest form, with the ion distribution taken as $f_i(v) = \delta(u-1)$, and neglecting the boundary conditions, the density of the charge-exchanged neutrals is given by

$$n_n(y) = n_+ v_+ / v_i a(\beta, j) \exp(-|jy|),$$

where j is the discrete eigenvalue obtained as the positive solution of the transcendental equation

$$1 - (\beta/2s) \ln[(1 + s)/(1 - s)] = 0,$$

and

$$a(\beta, j) = j^2 (1 - \sqrt{1 - \beta}).$$

This equation has roots $S = \pm j$, with $0 \leq j \leq 1$. For a given value of β , j is monotonic and can be readily computed. The quantity $a(\beta, j)$ is a slowly varying function of both parameters (see Refs. 27 and 28).

In the simplified form, a more exact solution for the neutral density for the slab with the simplified boundary conditions (in Eq. (7) only the neutral injection is taken into account) reads

$$n_n(y) = \int_0^\infty a(j) [\exp(y/j) + \exp(-y/j)] dj, \quad (17)$$

where

$$a(j) = \left[\operatorname{sgn}(j) \mu(j) F_+(j) + \beta F_i(j) P \int_{-\infty}^{+\infty} u F_+(u) / (j-u) du \right] / \\ \left[\left[\exp(a/j) + \exp(-a/j) \right] (u^2 + \beta j \pi F_i(j)) \right]^2,$$

and

$$\mu(j) = 1 - \beta P \int j F_i(u) / (j-u) du.$$

Here P stands for the Cauchy principal value. Although the solution (17) obtained by the method of singular eigenfunctions is not given as simple algebraic expressions, it is expressed as simple integrals involving a boundary condition which easily can be calculated numerically. So this approach avoids the need to solve an integral equation on each occasion as in numerical schemes. Models for diffuse and specular reflection of neutrals at the wall were discussed and an explicit solution was given for the case of specular reflection.

The main results in Ref. 25 were achieved for the neutral density profile. It was shown that if the mean-free path length for ionization significantly exceeds the one for charge exchange, the neutrals obey the diffusion law for $1 < x/\lambda_{\text{ch-ex}} < 2.39 (\lambda_i/\lambda_{\text{ch-ex}})^{3/2}$, where x is the distance from the wall, thus confirming results (20) obtained from fluid equations. Following the practice in the neutron transport theory, the solution obtained from the kinetics has been extrapolated to the boundary $x=0$ to provide for boundary conditions for the diffusion equation, which is a very difficult question for the fluid approach. The result reads

$$n(0) = 1.4 F_0 (1 + R_g) / (1 - R_g - R_d) v_+, \quad (18)$$

where $F_0 = \int f_+(v)dv$ is the flux of neutrals recombined at the wall, and v_+ is their injection velocity.

It was found that the density behaves as $n(x) \sim (\lambda/x)^{1/3} \exp[-3(x/2\lambda)^{2/3}]$ at large distances $x > 2.39 \lambda_i \sqrt{\lambda_i/\lambda_{ch-ex}}$, where λ is the total mean-free path. It implies a much slower rate of decrease as compared to the diffusion equation. The physical reason for this will be discussed later in connection with the form of the distribution function. This asymptotic solution can be used for testing the accuracy of numerical codes used to treat the neutral dynamics in tokamak transport codes. It was also found that the outward flux increases as the specular and the diffuse reflection coefficients increase.

This approach has been further extended by Burrell (29) who studied explicitly the validity of the diffusion approximation for arbitrary ionization and charge-exchange mean-free paths. It has been shown that the diffusion approximation is valid only for $\beta > 0.9$, which holds only for a plasma temperature $T < 6$ eV. It constitutes a rather stringent constraint and emphasizes that the diffusion approximation, though extremely convenient in its simplicity, should be used with great care. Two important parameters, the density and the average energy of neutrals, have been computed for different values of β . The average energy $\epsilon(y) = \int mv^2 f d^3v$ is the quantity that enters into the energy exchange between neutrals and plasma ions. The results are shown in Fig. 4. The diffusion solution is also plotted there. As discussed above it gives a good approximation only if β is close to unity. Moreover, there is a boundary layer of the order of the neutral mean-free path, where the diffusion solution falls for all values of β . The obvious reason for this is the violation of the assumption made in the diffusion theory that, in a layer close to the wall of such thickness, the source of neutrals is isotropized almost immediately.

An interesting observation is that the average energy of neutrals is larger than the plasma temperature in the center of the plasma of all values of β . It implies the over-estimation of the central ion temperature as deduced from the neutral energy spectra. On this basis the action of the plasma on neutrals is compared with speed filter. The reason for it is that the mean-free path of the neutral increases with its speed. Accordingly, those neutrals with a high speed born through charge exchange penetrate more deeply into the plasma than those with lower speed. Therefore, the neutral distribution function gets enriched by high energy particles. This enrichment

increases as ionization increases, i.e., β decreases, since ionization removes neutrals, while charge exchange isotropizes them. The low speed neutrals are therefore preferentially removed by ionization. Accordingly, the average energy of neutrals is larger than that of the ions in the inner area of the discharge. So, deep inside the plasma the neutral population may be interpreted as the flux of untrapped particles.

Recently, it was shown that the energy-dependent diffusion theory may describe neutral transport much better, and in its most advanced version, the multigroup diffusion theory provides the accuracy typical of the neutron kinetic theory (30). The reason is that in the one-group diffusion theory the usual assumption is that all the neutrals have the same distribution as plasma ions. This, of course, is not true in the vicinity of the source of neutrals (for example, close to the wall), since the source neutrals have a temperature different from the ions. However, if β is around unity, neutrals very quickly assume the temperature of the ions.

If β is not close to 1, ionization is appreciable, and the neutral particles will no longer assume the plasma velocity distribution. In fact, the distribution of the neutral particles will greatly deviate from the ion distribution, and only a multigroup theory will have a chance in this case. The multigroup diffusion theory with Marshak boundary conditions

$$f'(x_0) - k(1 - R)/(1 + R) f(x_0) = 0 ,$$

which are used to reproduce experimentally known values of the reflection coefficient on the boundary $x = x_0$ of the slab (k is the wave number), provides a good agreement with the results achieved from neutron kinetics, even for small values of β in an optically thin slab transparent to neutrals.

The same problem has been considered (31) from a completely different point of view. It has been noticed that the problem of the penetration of an oscillating electric field into a plasma, studied by Landau (32) using Laplace transform techniques, leads to an equation similar to Eq. (12). This similarity has been exploited by Volkov to discuss the neutral problem by analogy with the Landau treatment. The exact solution was obtained for the unrealistic case $R_s = 1$ and $R_d = 0$. An approximate solution was obtained for arbitrary values of surface coefficients. The results confirmed most of the conclusions of Connor (25). An estimate of the rate of neutral sputtering of

stainless steel was also made, resulting in values of 10^{-3} and 10^{-4} for the relative concentration of light and heavy impurities, respectively.

More recent work on the neutral dynamics has usually employed numerical methods of solution, often as part of a plasma transport code. Indeed, in plasmas with inhomogeneous temperature, numerical solutions appeared to be the only ones possible. The influence of the inhomogeneous ion temperature profile on neutral kinetics has been studied analytically by Igitchanov and Stakhanov (33) and Tandler (21). In the former work the diffusion approximation was employed, and only very small values of ion temperature gradients were allowed. In Ref. 21 the double delta function ion distribution was used for calculating the neutral density profile. It was shown that the nonuniformity of the ion temperature profile leads to important consequences for the neutral density profile. If the ion temperature profile gets steeper, the penetration depth for neutrals decreases. It was shown explicitly, by calculating distribution functions for incoming and outgoing neutrals, that this effect was due to the tail enrichment of the distribution of neutrals streaming toward the wall (outgoing), and a corresponding reduction, as compared to the local Maxwellian, in neutrals moving from the wall. The asymmetry results in the reduced penetration. It is important to account for this effect in using the neutral spectral measurements for ion temperature diagnostics. As sputtering by energetic neutrals is the main source of impurities from the first wall (though not from the limiter, where impurities are primarily sputtered by the ion flux), giving a lower limit for sputtering in a reactor, this enrichment is also an important effect in assessing the amount of impurities in a machine.

Very recently, their work has been extended by Bachmann (34) using the sophisticated mathematical method of the complex Fourier transformation. The solution of Eq. (14) was obtained under the rather general assumption that the Fourier transformation of the kernel $K(y)$ has to be rational. The explicit comparison of his solution with those given in Ref. 21 for the neutral density confirmed most of the results in the latter. The enhancement of the penetration coming from the hot plasma is slightly larger, and the penetration of neutrals coming from the wall is somewhat smaller than their calculations.

In conjunction with formulating the boundary conditions for the divertor plasma for the INTOR tokamak, two similar analytical approaches have been developed by Harrison et al. (35) and Volkov and Kirilov (36). The models are

capable of easily assessing the probability of an atom released from the wall recycling back to the wall as a "daughter" atom. Alternatively, the plasma albedo is calculated, which is an important parameter for formulating the appropriate boundary conditions for the plasma. Two regions were considered: the initial one, where an atom has a velocity v_+ characteristic of its release from a boundary surface, and a subsequent one, where the velocity has been changed by collision with a plasma proton, so that the "daughter" atom corresponds to a randomly directed particle with thermal velocity v_{th} . The plasma is assumed to be homogeneous and of infinite extent, and motion is considered only in the direction x normal to the surface.

Using a one-dimensional two-fluid approximation, the neutral distribution function was assumed to be a function of the inward flux, F_+ , (towards the hotter plasma) and outward flux, F_- , (towards the wall) only. Whether the neutral belongs to a particular flux may change only as a result of charge-exchange. In each charge-exchange collision a neutral either remains in the same flux category or is transferred to the other category with an equal probability. Ionization attenuates both fluxes. Thus

$$\pm \partial F_{\pm} / \partial x = -F_{\pm} / \lambda_i - F_{\pm} / \lambda_{ch-ex} + 1/2(F_+ + F_-) / \lambda_{ch-ex} \quad (19)$$

Equation (19), strictly speaking, applies only to the "daughter" atoms, which implies that $x > \lambda_{ch-ex}$. In order to incorporate the first region into this model, the value of the mean-free path for charge exchange corresponding to the inward flux F_+ , should be $\lambda_{ch-ex} = v_+ / n_e \langle \sigma v \rangle$, where v_+ is the velocity of cold neutrals, and v is the relative velocity between a cold neutral with velocity v_+ colliding with a plasma proton with thermal velocity.

Transforming Eq. (19) to equations for the sum $F_+ + F_-$ and difference $F_+ - F_-$, we obtain the simple second order differential equation

$$\partial^2 / \partial x^2 (F_+ + F_-) - (1 + \lambda)(F_+ + F_-) = 0 \quad , \quad (20)$$

where $\lambda^{-1} = \lambda_i / \lambda_{ch-ex}$ was assumed to be constant. Equation (20) can be easily solved both in the first and second regions and their solutions can be matched to provide for the continuity of fluxes. The results of their calculations are summarized in Fig. 5. Harrison et al. (35) arrived at the typical value 0.17 for the albedo for fast backscattered neutrals ($u = v_{th}$), and 0.3 for

slow neutrals ($u=0$). Volkov and Kirilov (36) have computed the enhancement factor, K , accounting for the cascade nature of charge-exchange processes and the albedo of the plasma. The parameter K is defined as the relation between the ratio of the ionization probability (trapped neutrals) to the probability for a neutral to return back to the wall, as a function of $1/\lambda$ (Fig. 5). It is seen to vary little as a function of temperature, ranging between 3 and 4.5. The scaling of the albedo with the ratio of mean-free paths, β , seems to coincide with the dependence $\sqrt{\beta}$ obtained by other authors.

B. Multiple Species Models

So far, all studies mentioned above were restricted to the one component of neutrals, namely, neutral hydrogen. However, the study of the kinetics of impurity neutrals is of basic importance in fusion research because of the problems of helium ash removal and impurity control during the quasi-steady-state operation of a thermonuclear reactor. With the recent progress in plasma confinement and heating, and the design studies of large toroidal devices such as INTOR aimed at alpha-particle production under fusion conditions, the problem of multicomponent neutral kinetics has gained significant interest.

One of the parameters which determines the concentration of impurities in a tokamak plasma is the permeability of the boundary region to neutral impurity atoms. For most impurity atoms the mean-free path lengths of neutrals are extremely short so that they are quickly ionized, and the resulting ions are transported along field lines back towards the limiter or a divertor plate to be pumped away.

There are some important exceptions to this general rule. Besides the hydrogenic neutral components of the main plasma, helium and oxygen are of special interest for fusion applications. Helium, a natural product of fusion reactions and also a minority component in the radio frequency heating schemes, has relatively long mean-free paths both for ionization and charge-exchange. Oxygen, which is the most common intrinsic impurity, has an accidentally resonant cross section for charge-exchange with protons, deuterons, and tritons. These peculiarities make the study of these elements far from trivial.

The ordering of the reaction rates is the important factor for assessing the neutral helium transport versus neutral hydrogen transport in a plasma.

In early studies it was argued that owing to much larger values of the charge-exchange cross section for hydrogen, an enhancement of the mean-free path length for ionization of hydrogen will take place. On the other hand, the neutral helium will gain much less energy from the ions because the charge-exchange cross section for collisions between helium atoms and ions is much smaller than for hydrogen, and the relative concentration of helium ions is expected to be very small (around one percent for a reactor) compared to hydrogen ions. Therefore, helium atoms, scattered mainly by elastic collisions on hydrogen ions in open configurations or by wall collisions in more closed schemes, seem to be slowed down by the inelastic collisions with the wall and ionized much more rapidly than the neutral hydrogen. In other words, plasma will act as a helium filter.

Lehnert (37) studied the transport of neutrals in a two-component plasma in connection with astrophysical applications. He showed that the ratio between the ion densities will, in general, differ from the ratio of densities for the two types of neutrals. In Ref. 38 is an analysis of the apparent element separation, but this study was limited to those situations where the relative abundance of the two elements in both the plasma and gas phase was constant across the layer. Owing to this doubtful assumption, significant element separation was predicted. His model has been reconsidered by Nocentini and Engelmann (39). They have shown that the steady states discussed in Ref. 38 represent only special situations of a much wider class of possible steady states. Further, in general, the density ratio of the two types of neutrals varies across the periphery, although the density ratio of the two types of ions remains almost constant. Fluid equations were used in these references for neutrals, and the diffusion approximation was employed.

The behavior of the plasma as a helium filter was reconsidered by Tendler and Chhabra (40) in order to assess the feasibility of the cool plasma mantle concept for the purpose of ash removal. Extending the kinetic approach for a one-component plasma, they have obtained analytical solutions for the distribution functions and the density profiles of both the neutral hydrogen and helium. The qualitative difference with the simple model of the helium filter arose due to another property of charge-exchange collisions besides the increase of the neutral average energy. Namely, charge-exchange collisions also lead to the effective isotropization of the neutral velocity distribution, so that their directed motion is lost very quickly at any plasma

temperature. Also complicating the picture are the lower ionization rate of helium compared to hydrogen, as well as the uncertainty of an effective injection velocity both for hydrogen (because a significant part of it is injected as molecules) and for helium (because of the lack of data on the interaction of helium with the material surfaces). The quantitative result of the study on the parametric dependencies was that no significant enrichment of helium should be expected, and the penetration depth for neutral hydrogen was found to be nearly equal for $T_{\text{plasma}} > 10$ eV, or slightly less for $T_{\text{plasma}} < 10$ eV, compared to helium neutrals. This result seems to be consistent with the experimental results of F-1 Stockholm (41), Doublet-III (42), and PDX (43), where no significant enrichments of helium have been observed. The measured values for the enrichment varied from 0.5 to 2 depending on the plasma profiles at the periphery.

The issue is even more complicated for oxygen, which is one of the most frequently encountered impurity species in tokamak discharges. The main reason is that the hydrogen charge-exchange rate with oxygen is of the same order of magnitude as the resonant charge-exchange rate for hydrogen with itself. The implications of this coincidental resonance phenomenon for tokamaks were first studied numerically by Cohen and Dylla (44). Recently, the same problem has been treated analytically by Tendler (45). This work emphasized additional complications arising from the fact that a significant part of the oxygen is desorbed from metallic surfaces as hydrogenic or metallic compounds. The oxygen thus passes through a sophisticated multistep evolution before arriving at the neutral atomic state. The basic result of this work is that a small fraction of oxygen neutrals are able to penetrate the plasma approximately as deeply as the neutral hydrogen. Thus oxygen released from the wall in the form of the oxygen compounds provides a source of fast and slow oxygen neutrals distributed over a large part of the edge region. Chhabra (46,47) has incorporated the effect of the radiative recombination into a transport model and has shown that it might affect the neutral population for a very dense plasma. The weakness of the analytical approach in this case lies in the assumption that the relative abundance of the first ionization stage of oxygen is a slowly varying function of optical thickness. This assumption is needed to keep the theory analytically tractable. Under real conditions, however, it is poorly met, except for the area around the top of a limiter or a high recycling region near a

neutralizing plate in a divertor. However, it does seem possible to extend the treatment to the case of the bell-shaped profile also.

We note, in conclusion, that when evaluating the role of analytical methods for neutral transport modelling, it should be kept in mind that while expected reactor power densities have been surpassed in tokamaks for quite a long time, reactor-relevant edge conditions with power fluxes larger than 300 W/cm^2 have not been reached so far on any device. So the extrapolation of present results to a reactor must rely upon untested scalings. Such scalings are more easily derived from the analytical models, provided their limitations are not directly violated in the experiments.

3. NUMERICAL METHODS

In contrast to the analytical methods described in Sec. 2, methods to solve Eqs. (12-14) numerically allow treatment of Maxwellian (and non-Maxwellian) plasmas, arbitrarily shaped temperature and density profiles, and detailed atomic and wall physical processes, simultaneously without any additional assumptions except that a one-dimensional geometry has to be used.

The assumption of one-dimensionality seems reasonable if a neutral code is attached to a one-dimensional plasma transport code. The first attempts to account for neutrals in a large plasma transport code in a self-consistent manner were undertaken by Duchs (48) using a fluid model. Since, however, at this time the mean-free paths were comparable with plasma dimensions, Duchs et al. (49-50) included the optical approach described in Sec. 2.

The standard method, suggested in Ref. 51, is to first solve Eq. (14) for the neutral density, and then, using the method of characteristics, to solve Eq. (12) for the neutral distribution function. To solve the integral equation

$$n_n(x) = \int K(x,y) n_n(y) dy + n_o(x) \quad , \quad (21)$$

where in the most general form

$$K(x,y) = \int f_i(x,t) \exp[-\tau(x,y,t)] / \lambda_{\text{ch-ex}}(x,t) (x-y)^2 dt \quad , \quad (22)$$

and τ is the optical depth from x to y

$$\tau(x, y, t) = \int_y^x \lambda(w, t)^{-1} dw.$$

Physically, $K(x, y)$ is the probability that a neutral from the point y will charge exchange at point x . Thus if we define

$$G(n) = \int K(x, y) n(y) dy,$$

then $n_1 = G(n_0)$ is the neutral density of the first generation of charge-exchange neutrals, $n_2 = G(n_1) = G^2(n_0)$ is the second generation density, and so on, and the sum of all generations is

$$n = n_0 + n_1 + n_2 + \dots = \sum G^i n_0. \quad (23)$$

One of the methods to solve Eq. (21) numerically is by an iterative algorithm which is computationally very fast. However, the number of iterations is a strong function of the zeroth-order approximation for the neutral density n_0 . For example, if n_0 is taken as the density of cold neutrals injected at wall temperature, more than 100 generations of charge-exchange neutrals are required to get convergence. On the other hand, if an analytical solution is used as a zeroth-order approximation, the number of iterations is reduced to 4-5 (51).

Another way to solve Eq. (21) is to discretize the system so that the operator G is a matrix multiplication of the source vector n_0 by a matrix K . Then it can be shown that the infinite sum in Eq. (23) converges to $(1 - K)^{-1}$, providing that $\|K\| < 1$, which holds in most of cases.

While these methods of solution do not show the explicit dependence of the neutral density on the plasma parameters as did the analytical solutions, they can be made computationally fast. This is how Eq. (21) was solved numerically in Ref. 23, 52-57. In the latter studies, the wall neutral source and the charge-exchange cross section were assumed to be nearly isotropic. This assumption is rather limited in validity, as discussed in Sec. 2.

The third alternative method to solve Eq. (21) is to approximate a solution by a finite expansion in terms of a set of basis functions satisfying the boundary conditions. The transformed equations are then converted to a set of algebraic equations with unknown coefficients, which are determined to provide for exact solution at some collocation points. The integration is

replaced by a finite summation approximating the integrals by an m-point Gauss-Legendre quadrature formula

$$\int_a^b f(x) = (b-a)/2 \sum_k w_k^{G-L} f(x_k) \quad ,$$

where w_k^{G-L} are the Gauss-Legendre coefficients.

The usual difficulty encountered in following this procedure is the singularity of the kernel of the integral K at the point $x=0$, so some care should be taken in using the transformation around this point. Problems also arise sometimes because neutrals are usually treated in a slab geometry while plasma profiles are calculated for cylindrical plasma. This fact can be taken into account by carefully imposing boundary conditions at the plasma center to provide for vanishing neutral and plasma fluxes there.

Most of the computational results mentioned so far have been presented in graphical form (usually on a log scale). A more accurate table form has been used by Garcia *et al.* (58) for the neutral density and flux in a slab geometry for several combinations of partially specular and diffuse reflection. The F_n method, developed by them to study basic transport problems in the fields of radiative transfer and rarefied gas dynamics, has been modified for the case of neutral transport. This method can be summarized as follows: First a system of singular integral equations for the distributions at the boundaries is established using quite general boundary conditions with arbitrary reflection coefficients. The exiting distributions are then approximated by a finite expansion in terms of a complete set of basis functions. The coefficients in the expansion are found by requiring that the set of integral equations be satisfied at certain collocation points. Once the boundary distributions are established, the method can be used to extend the solution to any location in the slab. The answers have been given in the form of tables for the neutral particle fluxes and densities as functions of parameters β , R_s , R_d , and the optical thickness. Different forms of ion distributions and energy reduction factors at the wall were considered.

An interesting observation is that the case of $\beta \sim 1$, which is the easiest to treat analytically, turns out to be the most difficult to study numerically. Another interesting point, taken up in Ref. 58 is the confirmation of the intuitive notion, already mentioned in Sec. 2, that the sensitivity of the integrated quantities, such as distribution functions of

fluxes, on the fine details of the input is much weaker than that of the neutral density, and much less computational effort is required to calculate the former. While the flux at the wall in the F_n method converges to five significant figures using less than 35 collocation points, a significantly higher number of the collocation points is required to obtain equally accurate values of the neutral density. The convergence is also the slowest close to the boundaries, where the analytical solution is the most easy to obtain.

Very recently numerical calculations of the density profiles of neutral hydrogen deuterium, tritium, helium, and oxygen in the boundary layers of a tokamak plasma have been performed by Goedheer (59). These profiles were obtained from the numerical solution of the integral equation for the neutral density. The integrals are represented according to the n collocating point Gauss-Legendre quadrature formula. The expressions for the density at the Gauss-Legendre abscissae then form a set of n linear equations from which the neutral density is obtained. Interpolation yields the density at any x coordinate. One of the interesting features of this work is the use of a new model for the relevant He cross sections recently developed at the Nagoya Institute of Plasma Physics.

Another interesting feature in Ref. 59 is the explicit comparison of the numerical results with corresponding ones obtained analytically (21,40,45). The agreement for the case of hydrogen seems to be quite satisfactory, although the dependence of the penetration depth on the ion temperature gradient turns out to be slightly weaker than predicted analytically. For the case of helium, the energy loss due to wall collisions was not taken into account, and therefore the significantly enhanced penetration of helium atoms has been reported. The importance of charge exchange with hydrogen was confirmed. A much deeper penetration of oxygen neutrals was computed in Ref. 59 when the charge-exchange processes were "switched on." However, these results are quantitatively more exact than the results obtained analytically, owing to approximations made in the latter and described before (Sec. 2).

Also recently Potters and Goedheer (60) predicted numerically a clear helium impoverishment for a mixture of helium with deuterium/tritium. The maximum value of the enrichment factor obtained by them is 0.3. However, they have neglected in their study the influence of a much lower injection velocity for helium neutrals than for hydrogen. Their conclusions may be altered significantly if the two-dimensional geometry of a divertor chamber is taken

into account as emphasized by Tokar (61).

4. MONTE CARLO METHODS

A. Introduction

Analytical and numerical approaches typically use geometric symmetries and simplified plasma parameters in order to make closed solutions. An alternative approach is to integrate the Boltzmann equation using Monte Carlo methods. Such methods provide very powerful tools for including the effects of asymmetric geometries and plasmas, and detailed atomic and wall physical processes. The analytic and Monte Carlo approaches are complimentary, with the analytic exposing explicitly dependences and scalings, while Monte Carlo techniques allow exploration of new parameter ranges and provide checks on the validity of analytic explorations.

Historically, applications of Monte Carlo method to the neutral transport problem (62-71) have all made use of modifications of techniques from neutronics codes. We describe here briefly the fundamentals. (For a more detailed description see Ref. 71.)

In order to see how the Boltzmann equation is solved using the Monte Carlo method, integrate Eq. (12') over u neglecting the recombination and assuming $f_n(y, u) = F(y)f_1(u)$ to get

$$\int_u u \frac{\partial f_n(y, u)}{\partial y} du + \int_u f_n(y, u) du = \beta \int_u f_1(u) du \int_v f_n(y, v) dv,$$

or

$$\frac{\partial F(y)}{\partial y} \int_u f_1(u) du + F(y) \int f_1(u) du = \beta \int_u f_1(u) du \times F(y) \int_u f_1(u) du,$$

which is just

$$\frac{\partial F(y)}{\partial y} = (\beta - 1) F(y), \quad (24)$$

since $\int f_1(u) du = \int u f_1(u) du = 1$. Equation (24) has the solution

$$F(x) = \exp\{-\gamma(x)\} = \exp\left[-\int dt/\lambda_{\text{tot}}(t)\right]. \quad (25)$$

We next derive Eq. (25) from a different point of view. Let $\xi(x)$ be the probability that a particle travels at least a distance x without making a collision. Then the probability of traveling at least a distance $x + dx$

without making a collision is

$$\xi(x + dx) = \xi(x) - \xi(x) dx / \lambda_{\text{tot}}(x)$$

which, solving for ξ , gives

$$\xi(x) = \exp[- \int^x dt / \lambda_{\text{tot}}(t)] \quad (26)$$

which is the same expression as Eq. (25).

The Monte Carlo method of solving the Boltzmann equation is then to track test flights using Eq. (26) to determine the distribution of collisions between neutrals and plasma. That is, given a uniform random variate ξ between 0 and 1 (URV), solve

$$\xi = \exp[- \int^{x(\xi)} dt / \lambda_{\text{tot}}(t)] \quad (27)$$

for the collision point $x(\xi)$. By running a sequence of test flights, a distribution of collision points is determined and, knowing the remaining terms in $C(f)$, such as plasma density and temperature and the reaction cross sections, we solve for the F in Eq. (25).

B. Test Flight Tracking

There are a number of methods of solving Eq. (27), all of which reduce to integrating

$$\int dt / \lambda_{\text{tot}}(t) \quad . \quad (28)$$

For example, assume that a test flight begins at x_0 with the velocity v_0 , and that the plasma region has been divided into two-dimensional zones with constant parameters (Fig.6). Choose a URV ξ and compute the first intersection, x_1 , of the flight path with a zone boundary, and set

$$d_1 = \exp[- \int_{x_0}^{x_1} dt / \lambda_{\text{tot}}(t)] \quad .$$

If $d_1 \geq \xi$, find the next intersection, x_2 , and set

$$d_2 = \exp\left[-\int_{x_1}^{x_2} dt/\lambda_{\text{tot}}(t)\right] .$$

If $d_1 d_2 \geq \xi$, continue until a point, x_n , is reached where $d_1 d_2 \dots d_n < \xi$. The solution, $x_c = x(\xi)$, is then between the points x_{n-1} and x_n . Since λ_{tot} is constant in the zone between x_{n-1} and x_n ,

$$d_c = \xi/(d_1 \dots d_{n-1}) = \exp[-(x_c - x_{n-1})/\lambda_{\text{tot}}],$$

and $x_c = x_{n-1} - \lambda_{\text{tot}} \ln(d_c)$.

The integral in Eq. (27) can also be integrated using the rejection method of integration (71,72). The main computational work in tracking by this method is in computing the neutral mean-free path length, λ . Computing λ requires only the knowledge of local plasma temperatures and densities. Thus it is easy to include continuously varying plasma parameters in the calculation. In the direct integration method above, however, the integral (Eq. 28) over the optical depth was made with a step function integrand, and the simple backing up to a solution after the final step's overshoot worked because the plasma quantities were assumed to be locally constant. Using the rejection method, however, the plasma parameters can be described by multidimensional polynomial fits, from which λ can be computed as a function of position.

C. Test Flight Weighting

Each test flight is given an initial statistical weight, w , which is the number of actual test flights it represents. As the test flight progresses through a sequence of collisions, this weight is reduced to account for attenuation by ionization. The weight w is reduced at each collision by the probability, β , that the collision was charge-exchange.

For example, after the first collision the test flight weight would be βw , with $(1-\beta)w$ atoms/sec having been ionized. This weight attenuation process continues until w is less than some preassigned minimum weight, w_{min} . At this point a choice is made between a pure charge-exchange, in which case w remains unchanged and the flight is continued, or a pure ionization, with w being set to 0 and the flight ended.

One subtlety of the charge-exchange process is that its cross section varies over the Maxwellian distribution of ion velocities (73). Thus the

choice of the velocity of the charge-exchanging ion must take into account the dependence of the reaction rate on the relative velocity between the ion and the neutral particle (64,69). Note that it is almost impossible to account for this effect in solving the problem either analytically or numerically.

D. Scoring

As we have seen, at each collision $(1-\beta)\omega$ particles ionize. The sum

$$s_j = \sum (1 - \beta)\omega \quad (29)$$

taken over all collisions in plasma zone j of all test flights represents the ionization rate in zone j . Dividing by the volume, V_j , of zone j , gives the local ionization rate density, $S_j = s_j/V_j$. Other rate densities are derived similarly. For example, the charge-exchange ion power loss in zone j is equal to

$$\sum \beta \omega (E_i - E_n) / V_j ,$$

where the sum is over all collisions in zone j , E_n is the energy of the incoming neutral, and E_i is the energy of the incoming ion.

The neutral density, n_n , in zone j is derived from the relation

$$S_j = n_n (n_e \langle \sigma_e v \rangle + n_i \langle \sigma_{ch-ex} v \rangle) ,$$

where the only unknown is n_n . We can also independently compute the average energy, $\bar{E}_n$, of neutrals being ionized in zone j

$$\bar{E}_n = \sum (1 - \beta) \omega E_n / S_j . \quad (30)$$

In regions containing no plasma we may assume a fictitious plasma of pseudo-ions, ψ , whose reaction

leaves H^0 completely unchanged. Taking the sum

$$s_j^\psi = \sum w \quad ,$$

over all collisions with pseudo-ions in zone j , the neutral density, n_{nj} , then obeys

$$S_j^\psi = s_j^\psi = n_{nj} \cdot n_{\psi j} \langle \sigma_{\psi v} \rangle \quad ,$$

where $n_{\psi j}$ is the pseudo-ion density in zone j , and $\langle \sigma_{\psi v} \rangle$ is the (artificial) rate coefficient of reaction (31). Note that the product $n_{\psi} \langle \sigma_{\psi v} \rangle$ should be taken so that the contribution to the total mean-free path length of the pseudo-ions is of the order of the scale length of the problem.

Wall fluxes, implantation, sputtering rates, and conductance probabilities can all be similarly computed by taking sums of test flights over collisions, in these cases with the walls. Again this option is a clear advantage of the Monte Carlo method, because exact wall geometries can be included in the calculation.

E. Wall Reflection Models

As mentioned in Sec. 2, the wall reflection model in an ideal neutral transport calculation would supply values for reflection coefficients, R_N , backscattered velocity distributions, and sputtering yields, for particles incident with a given energy, E_{in} , and angle, ϕ , on a surface of arbitrary roughness and composition. Three approaches to wall reflection modeling are:

1. Using simple energy and angle-dependent expressions such as the one found in Ref. 74:

$$R_N(E_{in}, \phi) = 1.0 + (1.0 - 2\phi/\pi)[R_N^0(E_{in}) - 1.0] \quad ,$$

where

$$R_N^0(E_{in}) = -0.237 \log_{10}(E_{in}/E_L) + 0.19 \quad ,$$

with E_L being the energy reduction constant. This approach is computationally fast but simplistic, and it does not fully exploit the power of the Monte Carlo method, where sampling from complicated

distributions can be easily made. However, analytic treatments of neutral transport do benefit from such realistic approximations expressed in this closed form.

2. Using reflection simulation codes such as TRIM (75) and MARLOWE (76) to create stored data sets of reflection coefficients and angular distributions for use in Monte Carlo codes. One drawback of this method is that the more distributions sampled in a Monte Carlo calculation, the larger the standard deviation for a given number of test flights. A second disadvantage is that statistical inaccuracies in the original data (both TRIM and MARLOWE themselves use Monte Carlo algorithms) will be forever present in data compilation.
3. Incorporating a reflection code, such as TRIM, directly into a Monte Carlo neutral transport code. This avoids the problem in method 2 of embedded inaccuracies. An additional advantage is that the projectile species and wall structure can be easily varied. However, the bad effect on the standard deviation of the results may be greater than in method 2. Further, the combined codes may be too costly to run.

F. Variance Reduction Methods

A measure of the level of confidence in the results from a Monte Carlo calculation is necessary in appraising the uncertainty of the calculation. A goal of any such algorithm is to be as efficient as possible, that is, to maximize the level of confidence in the results gained from a given number of test flights. A number of techniques, so-called variance reduction methods, are typically used.

One such method is the method of geometric splitting (72), which is used to amplify the number of scorings in selected regions. The entire geometry is divided into areas which are given weights corresponding roughly to the inverse of the expected probability that a test flight would reach them. For example, zones which are small in area, or isolated, or relatively far away from the start of a test flight, would be given higher weights than larger zones, or zones closer to the initial flight position. Flights which go from regions of lower weight into regions of higher weight are then split as follows by a predetermined factor $\rho > 1$: If ρ is an integer, then the

original test flight is replaced by ρ flights, each with a Monte Carlo weight $1/\rho$ of the original. The offspring flights then proceed independently, increasing the number of scorings in the more highly weighted region. More generally, in order to increase efficiency, the ascribing of weights to areas may be done according to the relative importance given to the area. Scorings may be increased through splitting in regions which could catch many flights even without splitting, if they are of the most interest.

Geometric splitting is the most efficiently used when combined with the method of Russian Roulette, where flights coming from a highly weighted region are selectively killed as they enter a region of less interest. They are killed with a given probability, with the weights of the surviving flights increased in order to preserve particles. Without this selection process, the split flights would eventually wander into regions of lesser interest, reducing the calculation's efficiency.

G. Grid Generation

The main input into multidimensional geometry problems is the description of the plasma and device geometries. Detailed two- and three-dimensional solutions for the plasma flux surfaces are obtained from MHD equilibrium codes. The results from such codes must first be converted into Euclidean coordinates, and then put into a grid form convenient to a Monte Carlo calculation (77). Coordinates of the more complex device structures, such as stellarators, can be determined by CAD (Computer Assisted Design) programs. The final step, and frequently the most difficult, is then to combine these descriptions of the plasma grid and the wall structure.

H. Vectorization and Multi-Processing Computers and the Monte Carlo Method

The level of confidence in the results from Monte Carlo calculations is roughly proportional to the square root of the number of test flights used in the calculation. Thus, decreasing the uncertainty in a result for a given algorithm by a factor of α requires an increase in computation cost of a factor of α^2 . Given such a cost/benefit ratio, development of new approaches to Monte Carlo calculations which rely on computer hardware and software is an active field of research.

Two somewhat complementary computer architectures designed for general large-scale scientific calculations have been introduced in the past few years

- pipeline/chaining computers, such as the Cray-1, CDC Cyber 205, and the Fujitsu M-380 and NAS 9060 machines, and multiprocessing computers such as the CRAY X-MP, CRAY-2, and the Fujitsu VP-200.

Pipeline/chaining, or vectorizing, machines use banks of registers to make the same calculation on sets of numbers using an assembly-line architecture in and between their arithmetic units (78). This architecture is optimal for computations which perform the same sequence of numerical operations repeatedly. Monte Carlo tracking schemes, however, typically employ many logical tests as they branch through the set of all possible test flight outcomes, destroying most of the order required to take fullest advantage of this computer architecture. Thus, in order to take advantage of vectorizing one must reorganize the calculation carefully, using efficient gather/scatter techniques.

A number of papers describing the vectorization of Monte Carlo algorithms in various physical fields have appeared in the past few years (78-80), and, in particular, in the field of neutral transport (81). Savings in computation times are typically factors of two to four for significantly vectorized codes.

Vectorizing involves a localized processing of events in parallel. A computer architecture which is more immediately applicable to linear Monte Carlo calculations is one containing multiple processors, each using a nonoverlapping copy of the flight tracking sub-algorithm to track test flights independently. Thus, on a computer with N processors, the flight tracking loop would be divided into N parallel loops, each computing 1/N-th of the calculation. The general literature on parallel computation is only beginning to appear (82). Reproducibility appears to be difficult to include in such algorithms when only a single random number generator is used. It appears that each processor will need its own generator.

5. SUMMARY

The most important immediate incentive for realistic neutral modelling is to predict the plasma performance in current experiments. However, it is not easy at present to choose experimental data that are direct measures of neutral transport. Some such parameters are plenum pressure, neutral emission spectrum, and so on. Unfortunately, even the best diagnosed machines have only a handful of sites available for direct measurement of these parameters, owing to problems of access, the need of ports for heating devices, and for

other diagnostics. Better coordination between the modellers and the experimentalists is certainly desirable to optimize the diagnostics designs of probes, pressure gauges, bolometers, spectrometers, etc., given the access restrictions. On the other hand, the experimental plasma parameters, such as density and temperature profiles, crucial to the overall confinement properties of a machine, are much less direct functions of the neutral transport. So the exact knowledge of the latter is required to minimize the necessity for juggling with physical models or including anomalous "effects."

If there were an adequate theory for the processes responsible for energy and particle transport in the plasma, then, for given boundary conditions, the plasma parameters at the periphery of a reactor could be calculated in a self-consistent way. Unfortunately, it is not the case, so that modelling of the boundary plasma in a reactor has to rely on empirical measurements in existing tokamaks. The question arises as to how such measurements are to be used, and even more importantly, how far they can be extrapolated. All modelling (including neutral modelling) becomes suspect if it yields values which are far outside the range obtained in current experiments.

The methods of neutral modelling have been divided into three groups: analytical, numerical, and Monte Carlo methods. Analytical methods are the most easy to extrapolate because the parametric dependencies are more easily observed from them. However, their validity is still rather restricted by some stringent constraints, such as assumptions of one dimensionality, special forms of the plasma profiles, simplified atomic physics and material physics data input. Further extension of the present models to consider simplified two-dimensional, divertor channel geometries and arbitrary plasma profiles, seems to be feasible and is highly desirable.

The rate of thermonuclear reactions is proportional to the product of the isotope ion densities, while the sum of those is restricted by the requirement of the stability of the plasma. On the other hand an excess of tritium neutrals around the material elements will result in the more stringent requirements on the pumping speed and complicate the problems of the tritium extraction from the material elements of a reactor. So, in order to model a reactor, more than one species of neutrals is required. The modelling of multispecies neutral transport by Monte Carlo methods has just started (83), and more work in this direction is required, in particular in application to the divertor geometry.

All numerical methods, both the direct solution of the Boltzmann equation and Monte Carlo, require data on atomic and wall physics which are as complete and accurate as possible. Unfortunately, the data need is far greater than what is presently available. So work in this direction is necessary, especially for the rough and dirty surfaces typical in current experiments.

The question of which computational method should be used for a given problem involves determining whether the added expense of a more complicated model is necessary to answer the relevant questions effectively. That is, how sensitive are the results for neutral density and temperature and dependent plasma source terms to the fine details of the models used? As a general rule, for cases with simple geometry such as open configurations or symmetric and small limiters, one-dimensional models seem to be satisfactory for describing neutrals. On the other hand, in the closed channels with pumping or in the vicinity of the limiting structures, two- and three-dimensional neutral particle distributions are preferable (see Table 2 and 3).

The methods described in Sec. 3 are computationally much faster than the Monte Carlo ones. For example, the code of Ref. 57 runs over 15 times faster than the comparable Monte Carlo code of Ref. 66 (0.3 CRAY-1 CPU sec and 5 CPU sec, respectively). It is certainly highly desirable to improve both the software and the hardware in order to cut further the computer times. Some work in this direction has been reported for both methods (60,70). Besides that, Monte Carlo methods are going to profit from the current development of a new generation of multiprocessor computers which will be ideally suited to linear Monte Carlo schemes.

In conclusion, the methods for modelling neutral transport have matured during the years through constant development, to the point where calculations can be performed in a reasonable fashion with reasonable accuracy. However, the experimental data necessary to compare with the results of the models are still sparse, and more interaction between them will be beneficial for both.

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Table 1
The Dominant Neutral/Plasma Reactions

Charge-exchange (H is any hydrogenic species):

Electron-impact ionization:

Ion-impact ionization:

Electron dissociation:

Recombination:

Table 2
Guidelines for Modelling

<u>Modelling Problem</u>	<u>Necessary Geometry</u>
High Recycling Divertor	1-D slab for parallel flow modeling 2,3-D for pumping efficiency
1-D Radial Plasma Transport	1-D Cylinder
1-1/2 D Radial Transport	2-D
Axisymmetric Divertor Problems: ASDEX-Upgrade, PBX, PDX, Big-D, JT-60	2-D
Bundle Divertor: DITE	3-D
Discrete limiters: TFTR, JET, TORE-SUPRA, FTU, etc.	3-D for data analysis
Pump-limiters: ISX, PDX Scoop, ALT-I and ALT-II	3-D
Stellarators: W-7, A1F, RFP	2-D and 3-D
Reverse field pinches: ZT-40M	2-D
Mirrors: TMX TFMX-B	1-D in the center cells and 2 and 3-D in end plugs
Non-circular Z-pinches: EXTRAP	2-D

Table 3
Some Widely Used Neutral Codes

<u>CODE</u>	<u>DIMENSIONALITY</u>	<u>NEUTRAL SPECIES</u>
SPUDNUT (53)	1-D slab	H
ANTIC (57)	1-D cylinder	Multiple H
MONET*(84)	1-D cylinder	H
AURORA/MONTE*(66)	1-D cylinder (can do ellipses)	Multiple H
DICON*(74,81)	2-D	Multiple H, H ₂ , and He
KUKUSHKIN AND PIGAROV*(85)	2-D	H, He
SEURAT*(86)	2-D	Multiple H
DEGAS*(69)	3-D	Multiple H, H ₂ , He, and CH _n
EIRENE*(67)	3-D	Multiple H, H ₂
NIMBUS*(64)	3-D	D/T, H ₂
GOEDHEER et al. (59)	1-D slab	D, T, He

* Monte Carlo codes

FIGURE CAPTIONS

- FIG. 1. The general outline of the different channels in neutral kinetics.
- FIG. 2. Results from Sacharov. Notice the different penetration for slow and fast neutrals.
- FIG. 3. Results from Zubarev and Klimov. The neutral densities of fast N_2 and slow neutrals N_1 versus the distance from the wall in mean-free paths.
- FIG. 4. Results from Burrell. The neutral energy is shown versus the optical thickness from the center. It is normalized to the plasma temperature. Notice the large difference in the neutral energy from the plasma near the wall (for all values of β) and in the inner core (for small β).
- FIG. 5. Results from Volkov and Kirilow. The parameter K is defined as the relation between the ratio of the ionization probability (trapped neutrals) to the probability of a neutral to return back to the wall, and the albedo of the plasma to the neutral particles versus λ^{-1} .
- FIG. 6. Tracking in two dimensions by integrating $\int ds/\lambda(s)$ directly. Starting at x_0 with velocity v , choose a uniform random variable ξ , $0 < \xi < 1$. The first intersection with the triangularized two-dimensional grid is at the point x_1 . If $\int_{x_0}^{x_1} ds/\lambda(s) < -\ln \xi$, the intersections $x_2, \dots$, are computed until $\int_{x_0}^{x_n} ds/\lambda(s) > -\ln \xi$, at which point the algorithm backtracks linearly to the point of collision $x(\xi)$.

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Fig. 1

Fig. 2

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Fig. 3

Fig. 4

Fig. 5

#84P0371

Fig. 6

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