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TEP/ICB Method for Neutral Particle Transport

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Abstract

Extensions of the transport/escape probabilities (TEP) and interface current balance (ICB) methods for neutral particle transport are presented. An evaluation of the accuracy of various assumptions made in the implementation of the methods is summarized. Comparison with Monte Carlo and an experiment in DIII-D are presented.

1 Introduction

We are developing a computationally efficient neutral particle transport methodology [1]-[3] based on the balance of partial currents across interfaces between contiguous regions in a multiregion representation of the plasma edge and divertor. The exiting partial currents across a surface bounding one part of a region are calculated as the sum of: 1) incident partial currents across other surfaces of the region which have been transmitted without collision to the surface in question; and 2) the exiting partial current arising from sources and from charge-exchange and elastic scattering events within the region. The transport is characterized by transmission and escape probabilities for the various regions, which depend on the region geometry, mean free path (temperature and density) distribution, and internal source and first collision source distributions. In implementing the methodology, a number of approximations are made in order to characterize the transport probabilities in terms of an average mean free path for a nonuniform region with nonuniform internal source distributions and to simplify the treatment of the angular distribution of the particles which constitute the partial currents across interfaces. One of the purposes of this paper is to report the results of an evaluation of the accuracy of these various approximations based on a detailed comparison with Monte Carlo and to present certain corrections which improve this accuracy. A further purpose of this paper is to report the comparison of TEP/ICP and Monte Carlo calculations and experimental results for neutral densities in the DIII-D edge plasma.

2 Transport methodology

ICB In 1D slab geometry, the forward (+) and backward (-) partial currents at the left (i) and right (i+1) interfaces bounding region i are related by [3]

$$\begin{bmatrix} J_i^+ \\ J_i^- \end{bmatrix} = \begin{bmatrix} (T_i^{-1}) & (-T_i^{-1}R_i^b) \\ (R_i^b T_i^{-1}) & (T_i - R_i^b T_i^{-1} R_i^b) \end{bmatrix} \begin{bmatrix} J_{i+1}^+ \\ J_{i+1}^- \end{bmatrix} + \frac{1}{2} s_i P_i \begin{bmatrix} -T_i^{-1} \\ 1 - R_i J_i^{-1} \end{bmatrix} \tag{1}$$

where the transport parameters are defined in terms of the exponential integral E_n

$$T_i = T_{oi} + R_i^f \, , \; T_{oi} = 2E_3(l_i) \, , \; R_i^{flb} = \Lambda_i^{flb} c_i P_i \left(1 - T_{oi}\right) \, , \; P_i = \frac{P_{oi}}{1 - c_i \left(1 - P_{oi}\right)}$$

$$P_{oi} = \frac{1}{2\Delta_i \sum t_i} \left[1 - 2E_3(l_i)\right] , \; c_i \frac{\langle \sigma v \rangle_{cx} + \langle \sigma v \rangle_{el}}{\langle \sigma v \rangle_{ion} + \langle \sigma v \rangle_{cx} + \langle \sigma v \rangle_{el}} , \; l_i = \int_0^{\Delta_i} dx \sum_{ti}(x) \equiv \Delta_i / \bar{\lambda}_i \tag{2}$$

The quantity T_{oi} is the probability that a particle is transmitted across region i without a collision and $c_i(1 - T_{oi})$ is the probability that an incident particle has a scattering or charge-exchange collision within the region. The quantity P_i is the probability that a neutral particle which enters region i across a given surface (i or i+1) and has an initial charge-exchange or scattering collision within region i will eventually escape from region i. Λ_i^b and $\Lambda_i^f = 1 - \Lambda_i^b$ are the relative probabilities that the escape is across the same or opposite, respectively, surface over which the incident particle entered the region. It was assumed that the local mean free path within the region could be approximated by an average mean free path for the region. If the further approximations are made that scattering and charge-exchange are isotropic and that the distributions of first-collided, second-collided, etc. particles are uniform over the region, then $\Lambda_i^f = \Lambda_i^b = 1/2$. R_i is evaluated for $\Lambda_i = 1/2$. The transmission probability, T_{oi}, is $E_2(l_i)$ for an incident plane source, $2E_3(l_i)$ for an isotropic incident flux, $3E_4(l_i)$ for a cosine incident flux, etc.

TEP The transport methodology is extended to 2D geometry by writing the partial current out of region i into region j, J_{ij}, in terms of the incident partial currents into region i from all contiguous regions k, J_{ki}, and the two-dimensional extensions of the transmission and escape probabilities defined previously

$$J_{ij} \; = \sum_k^i T_{oi}^{kj} J_{ki} \left[\sum_k^i \left(1 - \sum_m^i T_{oi}^{km} \right) J_{kj} \Lambda_{ij}^k \right] c_i P_i + s_i \Lambda_{ij} P_i \tag{3}$$

The transmission coefficients across region i for particles entering from region k and exiting into region j, in planar geometry with symmetry in the third dimension, are defined in terms of the Bickley functions Ki_n. The coordinate ξ_{ki} is along the interface between regions k and i, and $\phi_j(\xi_{ki})$ is the angle made with respect to the surface between regions k and i by a line connecting a point ξ_{ki} on that surface with a point on the surface between regions i and j

$$T_{oi}^{kj} \; = \; 2 \int_{\xi_{ki}^{min}}^{\xi_{ki}^{max}} d\xi_{ki} \int_{\phi_j^{min}(\xi_{ki})}^{\phi_j^{max}(\xi_{ki})} sin\phi_j \frac{Ki_3 \left(l_i \left[\phi_j \left(\xi_{ki} \right) \right] \right)}{\xi_{ki}^{max} - \xi_{ki}^{min}} \tag{4}$$

The escape probability can be written in terms of similar variables, but we choose for computation efficiency to use a rational approximation involving the average mean free path of the form

$$P_{oi} \; = \; \frac{1}{x_i} \left(1 - \left(1 + \frac{x_i}{n} \right)^{-n} \right) \, , \quad x_i \; \equiv \; \frac{4V_i}{S_i \bar{\lambda}_i} \tag{5}$$

where V_i and S_i are the volume (area in 2D) and surface area (circumference in 2D) of region i.

3 Accuracy of transport approximations & correction factors

The accuracy of the various approximations that are made in implementing the TEP/ICB transport methodology has been evaluated by comparison with the DEGAS [4] and MCNP [5] Monte Carlo codes.

First-Flight Transmission Probabilities First-flight transmission probabilities (FFTPs) calculated from Eq. (4) and with Monte Carlo were compared for regions with a variety of geometries bounded by straight lines and with an isotropically distributed incident flux. The agreement was essentially exact for uniform regions and for regions within which the density varied linearly. In regions within which the plasma temperature varied linearly within the range 1-100 eV, the use of an average mean free path resulted in errors in the FFTP of less than 1.5% for optically thin regions in which the FFTPs were greater than 70%, and in errors as large as 10% in optically thick regions in which the FFTPs were less than 5%. Thus, the error in the total transmission due to the error in calculating the fraction of incident particles which are transmitted without collision that is introduced by using an average mean free path to represent a nonuniform temperature distribution is less than 1%.

Escape Probabilities The rational approximation of Eq. (5) parameterizes the first-flight escape probability (FFEP) in terms of the single paramater $x = 4V/S\lambda$. Although this result follows from theoretical considerations [1],[6],[7], it was confirmed by fitting Monte Carlo calculated FFEPs for several geometries, volume-to-surface ratios and values of the mean free path. The original Wigner rational approximation [6] (n=1) is known to underestimate the FFEP in the midrange of x, and the Sauer rational approximation [7] (n=4.58) has been shown to be more accurate for an infinite cylinder (circle) geometry. For uniform media, we found that a new (n=2.09) rational approximation agreed with Monte Carlo calculations of the FFEP to within <5% for a wide range of geometries (excluding the circle), volume-to-surface ratios and mean free paths, but that the Sauer approximation was superior for circular regions. Calculation of FFEPs for regions in which the plasma density varied by as much as a factor of 20 and the plasma temperature varied over the range 1-100 eV demonstrated that Eq. (5) predicts the FFEP calculated by Monte Carlo to within <5% for nonuniform regions. Equation (2) indicates that the error in total escape probability will be less than the error in the FFEP.

Directional Escape Factors The theoretical development of the escape probability formalism assumes both uniform material properties and a uniform collision source within the region, and predicts only the total escape probability, without distinguishing directionality. Monte Carlo calculations of FFEPs for regions with temperatures varying across the region within the ranges 1-10 and 10-100 eV show a maximum directionality effect of less than 8% (e.g. the fraction escaping over any surface of a square differs from 0.25 by less than 8%). Monte Carlo calculations of an optically thick region with density variations of 2 and 20 produce maximum directionality effects of 1% and 25%, respectively.

In an optically thick region, the first collision source distribution of the incident partial current will be highly non-uniform, thereby producing a significant directional escape bias back across the incident surface. Monte Carlo calculations of this escape directionality effect for a range of mean free paths and region dimensions Δ can be represented by a fit to the ratio of the calculated forward (f) and backward (b) escape fractions, for regions with uniform properties. For two values of c_i, the values of c_1 through c_3 are

$$\frac{\Lambda_f}{\Lambda_b} = \frac{c_1}{1 + exp((y + c_2)/c_3)}, \quad y = \frac{\Delta}{\bar{\lambda}}, \quad \begin{array}{ccc} c_i & = 0.80 & 0.45 \\ \hline c_1 & 3.225 & 2.326 \\ c_2 & 1.145 & 0.268 \\ c_3 & 1.334 & 0.996 \end{array} \tag{6}$$

Interface Isotropization An 'isotropization' error is introduced by the assumption that the uncollided as well as the collided particles passing through successive interfaces have the same distribution within the forward hemisphere, for the purpose of calculating the transmission through successive regions. Thus, the calculation of the penetration of particles from a plane source at one surface of a multiregion problem contains two compensating errors: 1) the 'isotropization' error causes underprediction of penetration; and 2) the 'escape directionality' error (failure to account for predominant escape across incident surface) causes overprediction of penetration. Comparison with Monte Carlo indicates that for subdivision of the transport medium into regions of thickness greater than a mean free path, the second error is predominant, whereas the first error is predominant with subdivision into regions of thickness less than a mean free path, and the two errors almost exactly compensate for subdivision into regions of about one mean free path thickness. The escape probability directionality factor of Eq. (6) can be used to eliminate the second error.

4 DIII-D model problem comparison

A more definitive test of the efficacy of the TEP methodology (incorporated in the GTNEUT code) for fusion plasma analysis is provided by calculation of the DIII-D model shown in Fig. 1. A realistic plasma density distribution was modeled, and a uniform plasma and neutral temperature of 10 eV was used to evaluate cross sections [8] for both the GTNEUT and Monte Carlo (DEGAS [4]) calculations. As shown in Fig. 2, the GTNEUT results agree quite well with the DEGAS results near the recycling neutral sources at the divertor plates and in the lower divertor region, where most of the ionization takes place. There is about an order of magnitude disagreement, attributed to the interface isotropization error, in the upper part of the problem (DEGAS error bars ~10% at midplane, ~25% at top for 400,000 histories), where the ionization rate is down six to eight orders of magnitude relative to the divertor. The computational time required for the GTNEUT solution was about 1% of that required for the DEGAS solution.

5 Comparison with DIII-D neutrals measurements

A novel method was recently applied [9] in DIII-D to measure neutral densities at locations extending from 3.7 cm (private flux region) up through the X-point to 21 cm (well inside the separatrix) above the floor of the divertor. This experiment has been calculated, [10] using simple but comprehensive, coupled models of the SOL-divertor and core plasmas [11] and recycling neutrals, and using selected experimental

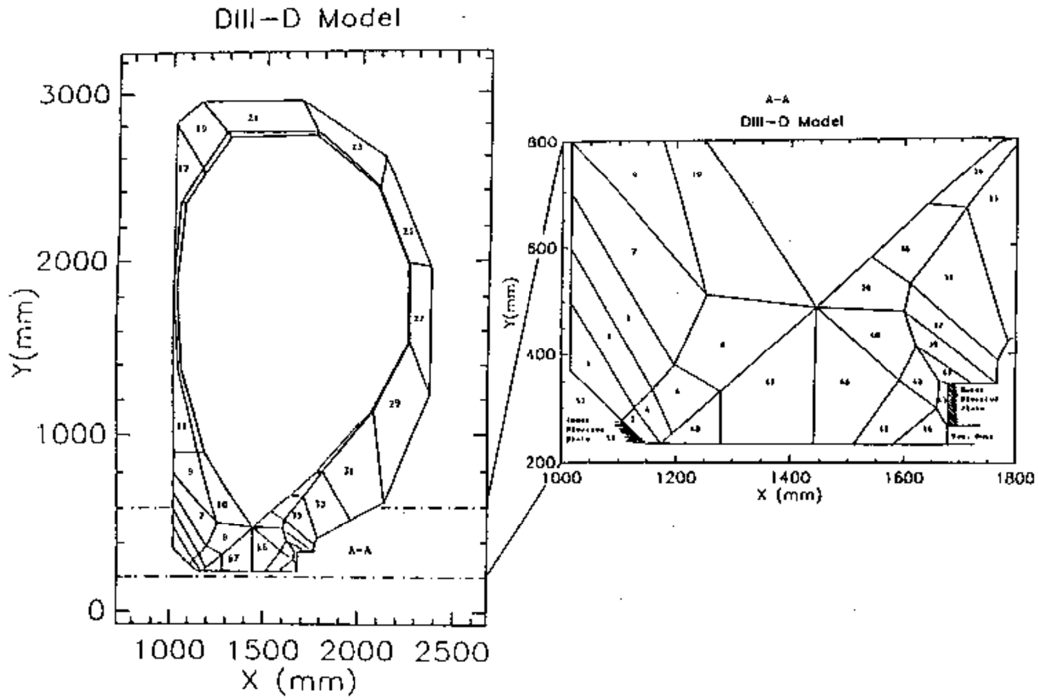

Fig. 1: Neutral atom transport model for the DIII-D plasma.

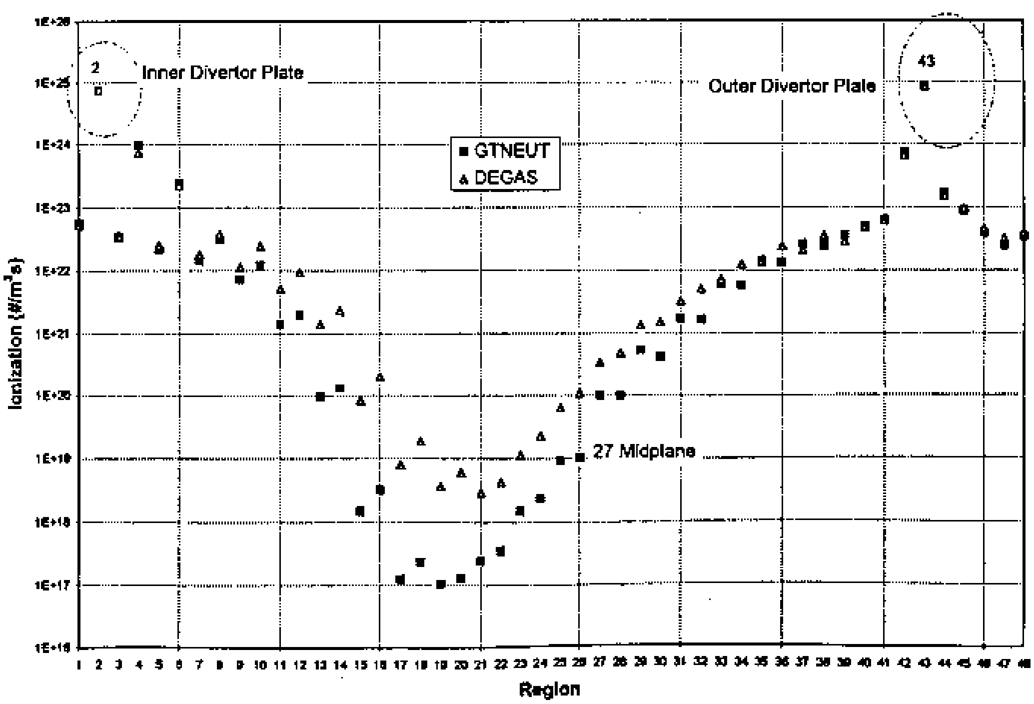

Fig. 2: Neutral atom ionization density distribution for DIII-D model problem.

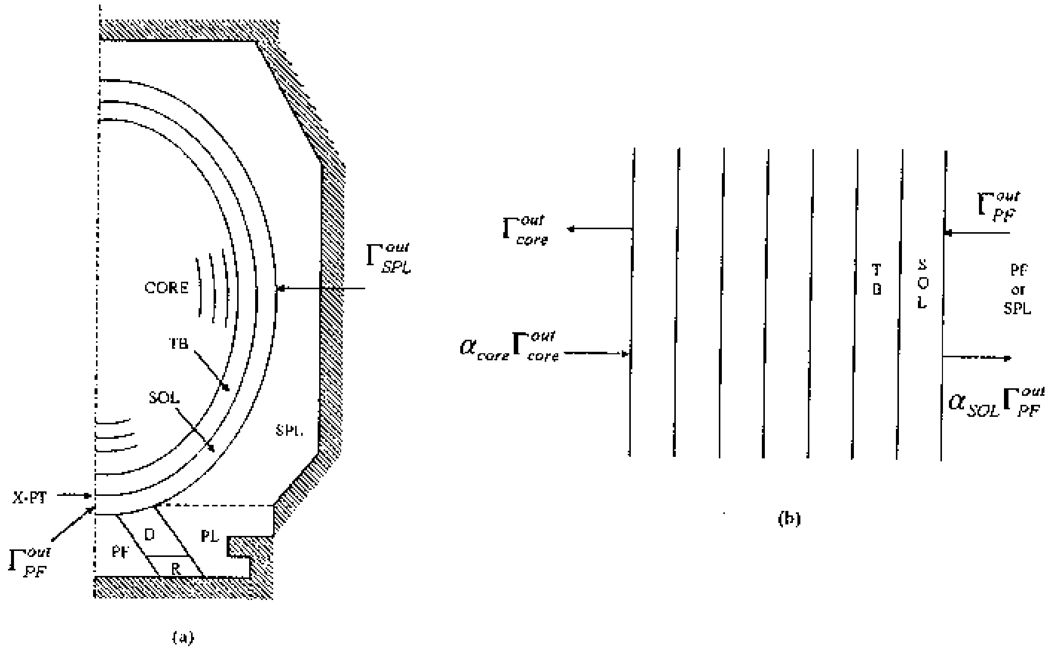

Fig. 3: Schematic of Neutral Transport Model: a) 2D TEP model of divertor plasma (D), recycling region (R), private flux (PF), plenum (PL) and scrape-off layer (SPL); and b) 1D ICB model of penetration through SOL and transport barrier (TB) into core.

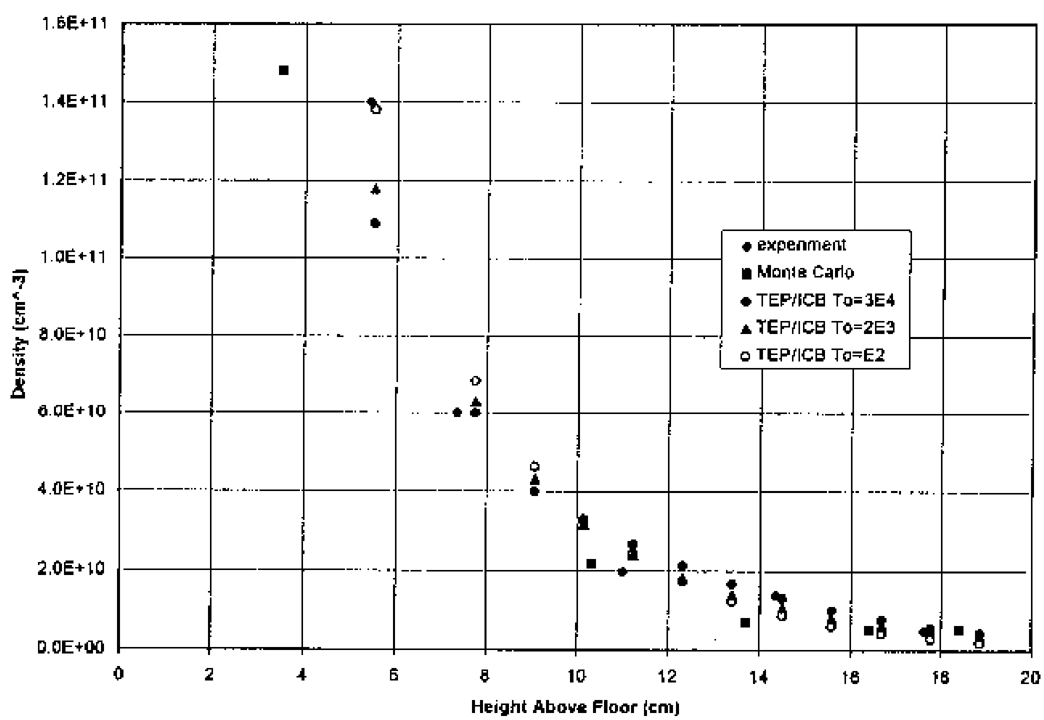

Fig. 4: Measured and calculated neutral densities in the lower part of the DIII-D plasma during shot 96740 at 4250 ms when the x-point was 7 cm above the divertor floor.

plasma data to insure fidelity of the background plasma representation. The neutrals model was a coupled TEP (for the 'outer' R, D, PF,PL and SPL regions) and ICB (for penetration inward across the separatrix into the edge plasma) model, as depicted in Fig. 3, with the neutral wall outgassing source adjusted to reproduce the measure line average density. The TEP/ICB results (for different T_o in the ICB model) are compared with the experimental data and with the results of a fluid plasma/Monte Carlo neutrals (B2.5/DEGAS) calculation [12] in Fig. 4. Both the TEP/ICB and Monte Carlo calculations agree quite well with the experimental data above the X-point The iterative background plasma and TEP/ICB neutrals calculations took less that one second on a PC.

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