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**A Two-Dimensional Finite Element
Multigroup Diffusion Theory
for Neutral Atom Transport in Plasmas**

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Mohammad Z. Hasan and Robert W. Conn

Mechanical, Aerospace
and Nuclear Engineering Department
Center for Plasma Physics and Fusion Engineering
University of California, Los Angeles
Los Angeles, California 90024

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ABSTRACT

Solution of the energy dependent diffusion equation in two dimensions is formulated by multigroup approximation of the energy variable and general triangular mesh, finite element discretization of the spatial domain. Finite element formulation is done by Galerkin's method. Based on this formulation, a two-dimensional multigroup finite element diffusion theory code, FENAT, has been developed for the transport of neutral atoms in fusion plasmas. FENAT solves the multigroup diffusion equation in X-Y cartesian and R-Z cylindrical/toroidal geometries. Use of the finite element method allows solution of problems in which the plasma cross-section has an arbitrary shape. The accuracy of FENAT has been verified by comparing results to those obtained using the two-dimensional discrete ordinate transport theory code, DOT-4.3. Results of application of FENAT to the transport of limiter-originated neutral atoms in a tokamak fusion machine are presented.

1. INTRODUCTION

The importance of the neutral atom distribution in a fusion plasma has long been recognized [1,2]. Neutral atoms influence the plasma particle and energy balance by undergoing ionization and charge exchange reactions in the plasma and by introducing high-Z impurity atoms through processes such as sputtering and impact desorption. Neutral atom sputtering of limiter/divertor components and vacuum vessel walls in a fusion device affect the lifetime of these components, in addition to the problem of impurity production and plasma contamination. Also, knowledge of the energy spectrum of neutral atoms emerging from the plasma can be used for diagnostic purposes, such as in the determination of the plasma ion temperature. Fluid plasma codes used to describe plasma behavior in tokamaks, such as WHIST [3] or BALDUR [4], use the results of neutral calculation as input to plasma simulation. For all these reasons, the accurate and efficient description of neutral atom transport in complex geometries is a key problem in fusion research.

In general, neutral atom transport has to be solved numerically because of the non-homogeneity or spatial variation of the plasma temperature and density. Several numerical solutions in one-dimensional geometry are available. Burrell [5] has developed the code, NEUCG, based on the solution of an integral equation for a one-dimensional cylindrical plasma. Audenaerde, Emmert, and Gordiner [6] have developed the one-dimensional slab geometry code, SPUDNUT, based on the numerical solution of an integral equation for the charge-exchange collision density. Hughes and Post [7] have written a one-dimensional cylindrical geometry code for neutral atom transport using the Monte Carlo method. Duchs et al. [8] solved for the neutral atom distribution in one-dimensional cylindrical plasma using a charge-exchange generation method, allowing up to 10 successive generations of charge-exchange

neutrals. Garcia et al. [9] numerically solved for the neutral atom distribution in a one-dimensional slab plasma and in a half-space using the F_N -method.

Neutral atom distribution in multidimensional plasma geometries have been obtained using the Monte Carlo methods. Heifetz et al. [10] and Reiter and Nicolai [11] have reported multidimensional Monte Carlo codes for neutral atom transport. Codes written specifically for neutron transport, such as ANISN [12], DOT-4.3 [13] and TRIDENT [14], can be used to calculate the distribution of neutral atoms in plasmas. Application of ANISN is reported in reference [15].

Often, a one-dimensional approximation of the fusion plasma is not realistic because there are localized sources of neutrals or because the geometry is not readily simplified. We have shown elsewhere [16,17] that energy dependent diffusion theory with P_1 -Marshak boundary conditions provides very good accuracy for the transport of neutral atoms in fusion plasmas. A two-dimensional diffusion theory code for the transport of neutral atoms will be much faster than transport theory and Monte Carlo codes. Therefore, the code FENAT has been developed based on the finite element solution of the energy dependent diffusion equation in X-Y cartesian and R-Z cylindrical/toroidal geometries. The energy dependence is treated by the multigroup method. In section II, the multigroup diffusion equation is written in (x,y,ψ) toroidal coordinates. Finite element formulation of the solution by Galerkin's method is treated in section III, and the solution of the resulting system of algebraic equations and the characteristics of the code, FENAT, are presented in section IV. Section V contains verification of the accuracy of FENAT and the results of sample calculations for neutral atom transport in the TEXTOR tokamak [18].

II. DIFFUSION EQUATION IN TOROIDAL GEOMETRY

The steady state energy and space dependent diffusion equation for neutral atom transport is

$$-\nabla \cdot D(\underline{r}, E) \nabla \phi(\underline{r}, E) + \sigma_t(\underline{r}, E) \phi(\underline{r}, E) = \int dE' \sigma_{cx}(\underline{r}, E' \rightarrow E) \phi(\underline{r}, E') + S_v(\underline{r}, E) \quad (1)$$

where $\phi(\underline{r}, E)$ is the total neutral atom flux, $D(\underline{r}, E)$ is the diffusion coefficient, $\sigma_t(\underline{r}, E)$ is the total plasma-neutral interaction cross-section (ionization plus charge exchange), $\sigma_{cx}(\underline{r}, E' \rightarrow E)$ is the charge exchange cross-section where a neutral atom with energy E' charge exchanges with a plasma ion of energy E , and $S_v(\underline{r}, E)$ is the volumetric source of neutral atoms. A common volumetric source would be recombination source which is important in high density plasma. Treating the energy dependence by the multigroup method, the group diffusion equation corresponding to Eq. (1) becomes [19,20]

$$-\nabla \cdot D_g(\underline{r}) \nabla \phi_g(\underline{r}) + \sigma_{t,g}(\underline{r}) \phi_g(\underline{r}) = \sum_{g'=1}^G \sigma_{g' \rightarrow g}(\underline{r}) \phi_{g'}(\underline{r}) + S_{v,g}(\underline{r}) \quad (2)$$

$$g=1,2,\dots,G$$

where g denotes a particular energy group. For P_1 -diffusion theory with isotropic charge exchange (scattering) cross-section, the diffusion coefficient D_g is given by $1/3\sigma_{t,g}$. In Eq. (2), $\sigma_{g' \rightarrow g}$ is the group to group charge exchange cross-section. Evaluation of these group cross-sections is discussed in ref. [21]. The multigroup cross-sections used here are calculated by the code PLASMX [21]. Equation (2) represents a set of G partial differential equations coupled by the first term in the right hand

side.

Equation (2) is valid for any coordinate system provided proper expressions are used for the gradient and divergence terms. This equation will now be written in the toroidal coordinate system (x, y, ψ) shown in Fig. 1. The metric (h_1, h_2, h_3) of this system is given by $h_1 = h_2 = 1$ and $h_3 = (R+x)$. Gradient and divergence terms in this system are [22]

$$\nabla A = \frac{1}{h_1} \frac{\partial A}{\partial x} \hat{x} + \frac{1}{h_2} \frac{\partial A}{\partial y} \hat{y} + \frac{1}{h_3} \frac{\partial A}{\partial \psi} \hat{\psi}$$

and

$$\nabla \cdot B = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial x} \left(\frac{h_2 h_3}{h_1} \frac{\partial B}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{h_3 h_1}{h_2} \frac{\partial B}{\partial y} \right) + \frac{\partial}{\partial \psi} \left(\frac{h_1 h_2}{h_3} \frac{\partial B}{\partial \psi} \right) \right]$$

where $\hat{x}, \hat{y}$ and $\hat{\psi}$ are the unit vectors in the respective directions of the toroidal coordinates (x, y, ψ) . Using these expressions in Eq. (2), with $A = \phi_g$ and $B = D_g \nabla \phi_g$, the group diffusion equation in toroidal coordinates (x, y, ψ) becomes:

$$-\frac{1}{(R+x)} \frac{\partial}{\partial x} (R+x) D_g \frac{\partial \phi_g}{\partial x} - \frac{1}{(R+x)} \frac{\partial}{\partial y} (R+x) D_g \frac{\partial \phi_g}{\partial y} - \frac{1}{(R+x)^2} \frac{\partial}{\partial \psi} (R+x) D_g \frac{\partial \phi_g}{\partial \psi} + \sigma_{t,g} \phi_g =$$

$$\sum_{g'=1}^G \sigma_{g' \rightarrow g} \phi_{g'} + S_{v,g} \quad (3)$$

When written in the toroidal coordinates (r, θ, ψ) , where $x = r \cos \theta$ and $y = r \sin \theta$, Eq. (3) becomes the same as that obtained by Pomraning and Stevens [23] by first writing the transport equation in (r, θ, ψ) and then taking the P_1 approximation of the angular flux to derive the P_1 diffusion equation.

With toroidal symmetry (i.e. ψ -symmetry), Eq. (3) becomes

$$-\frac{1}{(R+x)} \frac{\partial}{\partial x} (R+x) D_g \frac{\partial \phi_g}{\partial x} - \frac{\partial}{\partial y} D_g \frac{\partial \phi_g}{\partial y} + \sigma_{t,g} \phi_g = \sum_{g'=1}^G \sigma_{g' \rightarrow g} \phi_{g'} + S_{v,g} \quad (4)$$

— in domain Ω .

Without the factor $(R+x)$ Eq. (4) is the group diffusion equation in X-Y Cartesian coordinates, and with $(R+x)$ replaced by R and y by Z , it becomes the group diffusion equation in R-Z cylindrical coordinates. The boundary conditions considered for Eq. (4) can be written as:

$$J_{in}^g = S_0^g + \alpha^g J_{out}^g \quad (5)$$

where J_{in} and J_{out} are the scalar current of neutral atoms at the surface, S_0 is the surface source and α is the reflection coefficient for the neutral atoms from the wall material. Using the P_1 -Marshak expressions for J_{in} and J_{out} in Eq. (5) [20], the boundary conditions can be written after some algebra, as:

$$D \frac{\partial \phi_s}{\partial n} = \left(\frac{1-\alpha}{1+\alpha} \right) \frac{\phi_s}{2} - \frac{2S_0}{(1+\alpha)} \quad (6)$$

— on $\partial\Omega$, the boundary of the domain Ω .

where $\frac{\partial \phi_s}{\partial n}$ is the normal derivative of neutral atom flux at the surface. Special cases included in Eq. (6) are free surface boundary conditions ($\alpha=0$), reflection conditions ($\alpha=1$), and general albedo boundary conditions (α neither 0 nor 1). If there is no boundary source, $S_0=0$.

III. GALERKIN FORMULATION OF SOLUTION

Finite element solution of Eqs. (4) and (6) is formulated by Galerkin's method. Since the diffusion equation is self-adjoint, formulation by the variational method will result in the same equations as by Galerkin formulation. The group diffusion equation can be written in operator notation as

$$L\phi_g = q_g \quad (7)$$

where,

$$L \equiv -\nabla \cdot D \nabla + \sigma_{t,g}$$

$$\text{and } q_g \equiv \sum_{g'=1}^G \sigma_{g' \rightarrow g} \phi_{g'} + S_{v,g}$$

For clarity, the subscript or superscript 'g' will be dropped from now on except where ambiguity may arise. Let the neutral flux, ϕ , be approximated as:

$$\phi \approx [N] \{\phi\} \quad (8)$$

where,

$[N]$ = row vector of suitably chosen basis functions (functions of the spatial coordinates)

$\{\phi\}$ = column vector of unknown flux (nodal values)

In Galerkin formulation, the weak form of Eq. (7) is [24]

$$\int_{\Omega} [N]^T (L\phi - q) dV = 0$$

or,

$$-\int_{\Omega} [N]^T \nabla \cdot (D \nabla \phi) dV + \int_{\Omega} [N]^T q_t \phi dV - \int_{\Omega} [N]^T \left\{ \sum_{g'=1}^G \sigma_{g'} \nabla \phi_{g'} + S_v \right\} dV = 0$$

where $[N]^T$ is the transpose of $[N]$. The first term of the above equation can be simplified by using vector identity and Gauss' divergence theorem [17]. When this is done, the above equation becomes

$$\begin{aligned} \int_{\Omega} \nabla [N]^T \cdot D \nabla \phi dV - \int_{\partial \Omega} [N]^T D \frac{\partial \phi}{\partial n} dS + \int_{\Omega} [N]^T q_t \phi dV - \\ \int_{\Omega} [N]^T \left\{ \sum_{g'=1}^G \sigma_{g'} \nabla \phi_{g'} + S_v \right\} dV = 0 \end{aligned} \quad (9)$$

In two dimensions, the basis functions, N , are functions of x and y . Therefore, from Eq. (8),

$$\frac{\partial \phi}{\partial x} = \frac{\partial [N]}{\partial x} \{\phi\} \text{ and } \frac{\partial \phi}{\partial y} = \frac{\partial [N]}{\partial y} \{\phi\} \quad (10)$$

Let the domain Ω be divided into a finite number of subdomains or elements (triangular) as shown in Fig. 2. Then the integrals over the domain Ω and its boundary $\partial \Omega$ in Eq. (9) can be replaced by the sum of the integrals over the domain, Ω_e , of each element and over the boundary, $\partial \Omega_e$, of each boundary elements. Now using Eqs. (10) and (6) for $D \frac{\partial \phi}{\partial n}$ in Eq. (9) and writing out the gradient terms, the finite element equations for a single element, e , for the solution of the group diffusion equation, Eq. (4), in R-Z cylindrical/toroidal coordinates is obtained.

$$\begin{aligned}
& 2\pi \int_{\Omega_e} \frac{1}{(R+x)} \frac{\partial[N]}{\partial x} (R+x) D_e \frac{\partial[N]}{\partial x} \{\phi\}(R+x) dA_e + 2\pi \int_{\Omega_e} \frac{\partial[N]}{\partial y} D_e \frac{\partial[N]}{\partial y} \{\phi\}(R+x) dA_e \\
& + 2\pi \int_{\partial\Omega_e} \frac{1}{2} \left(\frac{1-\alpha}{1+\alpha} \right) [N]^T \phi_s(R+x) dL_e + 2\pi \int_{\Omega_e} [N]^T [N] \alpha_L \{\phi\}(R+x) dA_e = \\
& 2\pi \sum_{\alpha'=1}^G \alpha_{\alpha'} \int_{\Omega_e} [N]^T [N] \{\phi\}^{G'}(R+x) dA_e + 2\pi \int_{\Omega_e} [N]^T S_v^e(R+x) dA_e + \\
& 2\pi \int_{\partial\Omega_e} \frac{2S_o^e}{(1+\alpha)} [N]^T (R+x) dL_e \quad (11)
\end{aligned}$$

In Eq. (11), expressions for differential volume and surface elements (with toroidal symmetry), $dV_e = 2\pi(R+x)dzdy = 2\pi(R+x) dA_e$ and $dS_e = 2\pi(R+x)dL_e$ respectively, have been used. The integrations in Eq. (11) can be evaluated either analytically or numerically depending on the complexity of the known basis functions, $N(x,y)$. When this is done, we obtain an element matrix equation as

$$\underline{A}^e \{\phi\}^e = \{q\}^e \quad (12)$$

where $\underline{A}^e$ is a square matrix of size $(n \times n)$, n being the number of unknown nodal values in the element, e . Matrix representation for the whole domain Ω and its boundary $\partial\Omega$ is obtained by properly adding Eq. (12) for all the elements in the domain, Ω . To obtain explicit expressions for $\underline{A}^e$ and $\{q\}^e$, we need basis functions, $N(x,y)$.

Let the neutral flux ϕ be represented by a linear polynomial in an element, e ,

$$\phi = \alpha_1 + \alpha_2 x + \alpha_3 y \quad (13)$$

with nodal conditions:

$$\phi = \phi_1 \text{ at } x = x_1, y = y_1$$

$$\phi = \phi_j \text{ at } x = x_j, y = y_j$$

$$\phi = \phi_k \text{ at } x = x_k, y = y_k$$

By inserting these conditions in Eq. (13), one finds α_1 , α_2 and α_3 . Then ϕ can be written as [25]

$$\phi = [N] \{\phi\} = N_1 \phi_1 + N_j \phi_j + N_k \phi_k$$

where the basis functions are

$$N_1 = \frac{1}{2A} (a_1 + b_1 x + c_1 y)$$

$$N_j = \frac{1}{2A} (a_j + b_j x + c_j y)$$

$$N_k = \frac{1}{2A} (a_k + b_k x + c_k y)$$

Here, A is the area of the triangular element with vertices i, j, k read counterclockwise and a, b and c 's are constants determined by the nodal coordinates. The integrals in Eq. (11) can be evaluated analytically with linear polynomial in Eq. (13). Use of higher order polynomials would require numerical integration. If the side $j-k$ of an element belongs to the boundary $\partial\Omega$, then the expression for ϕ on this boundary side becomes

$$\phi_s = \phi_{jk} = [N] \{\phi\} = [0 \ N_j \ N_k] \begin{bmatrix} \phi_1 \\ \phi_j \\ \phi_k \end{bmatrix}$$

since $N_i = 0$ on $j-k$, and similarly for the other two sides if they also belong to the boundary.

Inserting these expressions for the basis functions and their derivatives

in Eq. (11) and evaluating the line and area integrals, we obtain the expressions for $\underline{A}^e$ and $\{q\}^e$ in Eq. (12). For R-Z toroidal/cylindrical geometry, these are:

$$\underline{A}^e = 2\pi\bar{X} \frac{D_e}{4A_e} \begin{bmatrix} b_i^2 & b_i b_j & b_i b_k \\ b_i b_j & b_j^2 & b_j b_k \\ b_i b_k & b_j b_k & b_k^2 \end{bmatrix} + 2\pi\bar{X} \frac{D_e}{4A_e} \begin{bmatrix} c_i^2 & c_i c_j & c_i c_k \\ c_i c_j & c_j^2 & c_j c_k \\ c_i c_k & c_j c_k & c_k^2 \end{bmatrix} +$$

$$2\pi\alpha_t^e A_e \begin{bmatrix} d_1 & e_1 & e_2 \\ & d_2 & e_3 \\ \text{sym.} & & d_3 \end{bmatrix} + 2\pi\left(\frac{1-\alpha}{1+\alpha}\right) \frac{L_{ij}^e}{24} \begin{bmatrix} (3X_i+X_j) & (X_i+X_j) & 0 \\ (X_i+X_j) & (X_i+3X_j) & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (14)$$

where $\bar{X} = (X_i + X_j + X_k)/3$. The last term in Eq. (14) arises when the side i-j belongs to the boundary, $\partial\Omega$. If the element is not a boundary element, this term would be absent. If j-k or k-i is the boundary side, then the last term in Eq. (14) would respectively be

$$2\pi\left(\frac{1-\alpha}{1+\alpha}\right) \frac{L_{jk}^e}{24} \begin{bmatrix} 0 & 0 & 0 \\ 0 & (3X_j+X_k) & (X_j+X_k) \\ 0 & (X_j+X_k) & (X_j+3X_k) \end{bmatrix}, \text{ or}$$

$$2\pi\left(\frac{1-\alpha}{1+\alpha}\right) \frac{L_{ki}^e}{24} \begin{bmatrix} (3X_i+X_k) & 0 & (X_i+X_k) \\ 0 & 0 & 0 \\ (X_i+X_k) & 0 & (X_i+3X_k) \end{bmatrix}$$

where,

$$\begin{aligned} d_1 &= (3X_i + X_j + X_k)/30 & e_1 &= (2X_i + 2X_j + X_k)/60 \\ d_2 &= (X_i + 3X_j + X_k)/30 & e_2 &= (X_i + 2X_j + 2X_k)/60 \\ d_3 &= (X_i + X_j + 3X_k)/30 & e_3 &= (2X_i + X_j + 2X_k)/60 \end{aligned}$$

$L_{ij}^e, L_{jk}^e, L_{ki}^e$ are the lengths of the respective side of the triangular element, e .

And,

$$\{q\}^e = 2\pi \sum_{g'=1}^G \sigma_{g'} \cdot g' A_e \begin{bmatrix} d_1 & e_1 & e_1 & \phi_1 \\ & d_2 & e_3 & \phi_j \\ \text{sym.} & & d_3 & \phi_k \end{bmatrix} g' + 2\pi S_v^e A_e \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} +$$

$$2\pi S_o^e L_{ij}^e \begin{bmatrix} \frac{X_i}{3} + \frac{X_j}{6} \\ \frac{X_i}{6} + \frac{X_j}{3} \\ 0 \end{bmatrix} \text{ or } 2\pi S_o^e L_{jk}^e \begin{bmatrix} 0 \\ \frac{X_j}{3} + \frac{X_k}{6} \\ \frac{X_j}{6} + \frac{X_k}{3} \end{bmatrix}$$

$$\text{or } 2\pi S_o^e L_{ki}^e \begin{bmatrix} \frac{X_i}{3} + \frac{X_k}{6} \\ 0 \\ \frac{X_i}{6} + \frac{X_k}{3} \end{bmatrix} \quad (15)$$

where,

$$u_1 = (2X_i + X_j + X_k)/12$$

$$u_2 = (X_i + 2X_j + X_k)/12$$

$$u_3 = (X_i + X_j + 2X_k)/12$$

It can be seen from Eq. (14) that the element matrix $\underline{A}^e$ is symmetric, diagonally dominant and positive definite. When the Eqs. (14) and (15) are properly summed over all the elements in the domain Ω , we obtain the global matrix representation of the nodal values of the neutral flux, ϕ .

$$\underline{A} \{\phi\} = \{q\} \quad (16)$$

The global matrix has evidently the above mentioned properties. In the next section we discuss the solution of the matrix Eq. (16) and general characteristics of the code, FENAT, which is based on this solution.

IV. SOLUTION OF THE FINITE ELEMENT EQUATIONS

An equation similar to Eq. (16) exists for each energy group. These equations are coupled through the right hand side $\{q\}$ which contains the charge-exchange (scattering) source term. At each iteration over the energy groups, the right hand side $\{q\}$ for each group must be recalculated from the most recent group fluxes. The global matrix $\underline{A}$ is fixed for a specific discretization of the domain Ω . Hence, we have, for each energy group, a matrix equation where the matrix $\underline{A}$ is fixed but the right hand side is changing. Since the matrix $\underline{A}$ is diagonally dominant and positive definite, convergence and stability of the solution of Eq. (16) is guaranteed. The matrix $\underline{A}$ is banded and sparse. The bandwidth depends on the problem size and the way of numbering the nodes.

There are two major groups of methods for solving this set of equations. These are the direct or elimination methods and the iterative methods. A survey of available elimination and iterative methods is available elsewhere [25-29]. It is a unanimous view in the structural mechanics community that the iterative methods cannot compete with the elimination methods, especially for problems with multiple right hand sides [25-27]. As mentioned above, the right hand side of Eq. (16) changes because of the charge exchange source term in it. Therefore, an elimination method has been selected to solve the set of Eq. (16). This method is based on the column profile storage of the global matrix $\underline{A}$ and its L-U decomposition by Crout variation of Gauss elimination [27].

The code developed based on the above solution method for the transport of neutral atoms in fusion plasmas is called FENAT, an acronym for Finite Element Neutral Atom Transport. It is written for use on CRAY computers. Solution can be obtained in X-Y cartesian and R-Z cylindrical/toroidal geometries. Dynamic memory allocation is provided. Hence, small problems will require short clock-time for running. Various plotting options such as spatial mesh plot in its entirety or in a specified number of windows, 3-D total neutral atom flux, density and average energy plots, variation of total density and average energy as functions of poloidal angle and plasma radii as parameters, contour plot of total density, and plots of wall-material sputtering, erosion rate and power deposition as functions of poloidal angle are provided. Figure 3 is a simplified flow chart for FENAT. Detailed information for running the code is provided in a User's Manual [30].

V. VERIFICATION OF FENAT AND ITS APPLICATION TO TEXTOR TOKAMAK

Accuracy of FENAT has been assessed by comparing it with the two-dimensional transport theory code DOT-4.3 [13]. Figure 4 compares the results of FENAT with those of DOT-4.3. The problem is a 20 cm by 20 cm square plasma in cartesian coordinates. Neutrals at the top, bottom and right surfaces are reflected while the left surface is subject to a vacuum boundary condition. A surface source of neutrals is localized at $x = 20$ cm and $y = 8$ cm to 14 cm. In Fig. 4(a), the medium is homogeneous with the scattering to total cross-section ratio, c , equal to 0.8 and the mean free path is 4 cm. This is a one-group solution. In Fig. 4(b), the medium is plasma with the following properties:

$$T_i(0) = T_e(0) = 1 \text{ KeV}$$

$$T_i(20) = T_e(20) = 50 \text{ eV}$$

$$n_i(0) = n_e(0) = 5 \times 10^{13} \text{ cm}^{-3}$$

$$n_i(20) = n_e(20) = 1 \times 10^{12} \text{ cm}^{-3}$$

energy of source neutrals, a few eV.

Plasma properties are uniform along y. Temperature and density profiles are assumed parabolic. The flux in Fig. 4(a) and total density in Fig. 4(b) are shown as functions of x at y = 2cm and y = 10cm. Figure 5 compares the total neutral density by FENAT and DOT-4.3 for R-Z toroidal geometry with 20cm by 20cm square cross-section. The boundary and source conditions and the plasma properties are similar to those in Fig. 4(b). Both Figs. 4 and 5 show that FENAT is quite accurate compared to the transport theory. For the cases in Fig. 4(b) and Fig. 5, FENAT is about 62 and 96 times faster than DOT-4.3 respectively. It appears that the transport theory code converges rather slowly when there is complete up-scattering and down-scattering in the multigroup cross-section as is the case for plasma-neutral interactions.

FENAT has been applied to calculate the distribution of limiter-originated neutral atoms in the TEXTOR tokamak plasma [31]. Figure 6 shows the TEXTOR geometry. Figure 6(a) shows a cutaway view of the vacuum vessel with the toroidal belt limiter, ALT-II [18] in place. Figure 6(b) shows a cross-sectional view of the vacuum vessel. The limiter is located in the fourth quadrant centered at 45° and is a localized source of neutral atoms due to the recycling of neutralized plasma ions from the limiter surface. The neutral source is 22 times larger at the limiter tips than at the rest of the limiter surface. Table I contains the TEXTOR parameters and the plasma properties. The reflection coefficients are calculated from ref. [32]. All neutral atoms not reflected directly from the wall are assumed to desorb and

reenter the plasma with a few eV of energy. Fifteen energy groups up to the maximum energy of 3 keV have been used.

Figure 7 shows the spatial mesh plotted in four windows. The boundary elements marked by 's' represent the limiter (surface source). Total neutral atom density is shown in the 3-D plot in Fig. 8. The two peaks correspond to the tips of the limiter. A 3-D plot of average neutral energy is shown in Fig. 9. Figure 10 shows the average energy plotted as a function of poloidal angle at five plasma radii. Figures 9 and 10 show that the average energy of the neutral atoms is low near the plasma edge and higher and flat towards the center of the plasma. This is due to the well-known fact that plasma acts as a filter for low energy neutrals so that the energy spectrum of neutral atoms becomes harder as one proceeds towards the center of the plasma. The plasma is optically thin for high energy neutrals. In this problem, there are 1886 nodal points (unknowns), 3640 triangular elements and 15 energy groups. The computation time is about 2 minutes on the CRAY-1 (D-Machine).

VI. SUMMARY

A two-dimensional code, FENAT, for the transport of neutral atoms in fusion plasmas has been developed based on the solution of the multigroup diffusion equation using the finite element Galerkin method. Geometries allowed are X-Y cartesian and R-Z cylindrical/toroidal. The use of the finite element method allows solutions to be obtained in arbitrary cross-sectional geometries, such as D-shaped tokamak plasmas. Comparison with the transport theory code DOT-4.3 has shown that FENAT is quite accurate and much faster than DOT-4.3. It is expected that FENAT will be even faster when compared to Monte Carlo codes. FENAT has also been applied to TFTR tokamak. These results are reported elsewhere [33].

Localized neutral atom sources, such as limiter-originated neutrals in

tokamak problems, lead to neutral atom density and wall effects that are strong functions of poloidal angle. In such cases, results from one-dimensional (slab or cylindrical) solutions of neutral atom distribution will be inadequate for the calculation of neutral-wall interaction effects and for use in fluid plasma codes. Neutral atom distributions from a 2-D or 3-D neutral atom transport code can be used in plasma simulation codes such as WHIST [3] or BALDUR [4]. The use of diffusion theory will yield accurate solution with considerably greater speed. The FENAT code is the first step in this direction and can be used in conjunction with two-dimensional plasma modelling codes.

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Table I: TEXTOR Parameters and Plasma Properties

Major radius	175 cm
Minor radius	48 cm
Plasma cross section	circular
Limiter material	graphite
First-wall material	stainless steel (assumed iron)
Central plasma ion temperature	0.773 keV
Central plasma electron temperature	0.865 keV
Edge plasma ion temperature	50 eV
Edge plasma electron temperature	100 eV
Central plasma density	$2.5 \times 10^{13} \text{cm}^{-3}$
Edge plasma density	$8.4 \times 10^{12} \text{cm}^{-3}$
Total plasma ion efflux rate	$6.0 \times 10^{21} \text{sec}^{-1}$

Parabolic temperature and density profiles are assumed.

List of Symbols

Capital English Letters:

$A, \underline{A}, \underline{A}^e$

$D(\underline{r}, E), D_{\underline{g}}(\underline{r})$

E

G

J_{in}^g, J_{out}^g

L_{ij}, L_{jk}, L_{ki}

$\{N\}, [N]^T; N_i, N_j, N_k$

R

$S_v(\underline{r}, E), S_{v,g}(\underline{r}), S_o^g$

T_i, T_e

X, Y, Z

$X_i, X_j, X_k; Y_i, Y_j, Y_k$

$\overline{X}$

Small English Letters:

a_i, a_j, a_k

u_1, u_2, u_3

b_i, b_j, b_k

x, y

c_i, c_j, c_k

$\hat{x}, \hat{y}$

d_1, d_2, d_3

e_1, e_2, e_3

e

h_i, h_2, h_3

n_i, n_e

$\{q\}, \{q\}^e$

$\underline{r}$

Capital Greek Letters:

$\{\phi\}, \{\phi\}^e$	(phi)
ϕ_i, ϕ_j, ϕ_k	
Ω, Ω_e	(omega)
$\partial\Omega, \partial\Omega_e$	(del-omega)
Σ	(sigma)
$\Psi, \hat{\Psi}$	(psi)

Small Greek Letters:

α, α^g	(alpha)
$\alpha_1, \alpha_2, \alpha_3$	(alpha)
$\phi(\underline{r}, E), \phi_g(\underline{r})$	(phi)
$\phi_g(\underline{r}), \phi_s$	
θ	(theta)
π	(pi)
$\sigma_t(\underline{r}, E), \sigma_{t,g}(\underline{r})$	(sigma)
$\sigma_{cx}(\underline{r}, E' \rightarrow E), \sigma_g, \sigma_g(\underline{r})$	
∂	(del)
∇	(nabla)

Legends for Figures

- Figure 1: Toroidal coordinates, (x, y, ψ) .
- Figure 2: (a) Discretization of the domain, Ω , into triangular elements.
(b) The nodal conditions at the nodes i, j, k .
(c) An element with one side belonging to the boundary, $\partial\Omega$.
- Figure 3: A simplified logical flow diagram for FENAT.
- Figure 4: Comparison of neutral flux ($\text{cm}^{-2}\text{sec}^{-1}$) and total neutral density by DOT-4.3 and FENAT for 2-D X-Y geometries. DOT to FENAT CPU time ratio is about 4 in case (a) and about 62 in case (b).
- Figure 5: Comparison of total neutral atom density by FENAT and DOT-4.3 for 2-D R-Z toroidal geometry. DOT to FENAT CPU time ratio is about 96.
- Figure 6: TEXTOR geometry with ALT-II limiter.
(a) Cutaway view of the TEXTOR vessel.
(b) TEXTOR cross-section showing the location of the limiter, ALT-II.
- Figure 7: FENAT spatial mesh for TEXTOR geometry. The mesh is plotted in 4 windows. Elements marked by "s" represent the limiter (surface source).
- Figure 8: 3-D plot of total neutral atom density in TEXTOR by FENAT. The maximum total density is normalized to 10^{10} cm.
- Figure 9: 3-D plot of average neutral atom energy (eV) in TEXTOR by FENAT. Low energy near the edge is due to the filtering of the wall-originated low energy neutral atoms by the plasma towards the plasma edge.
- Figure 10: Variation of average neutral atom energy along the poloidal direction at five plasma radii. The limiter is located between 297 and 333 degrees.

$$\begin{aligned} X &= (R+x) \cos \psi & \text{-Cartesian } (X, Y, Z) \\ Y &= (R+x) \sin \psi & \text{-Toroidal } (x, y, \psi) \\ Z &= y \end{aligned}$$

3-D TOTAL DENSITY PLOT

3-D AVERAGE ENERGY PROFILE