JOURNAL OF COMPUTATIONAL PHYSICS **26**, 80–86 (1978)

A Method to Solve the Impurity Diffusion Equation with Ionization and Recombination Source Terms

MASAO OKAMOTO

Division of Thermonuclear Fusion Research, Tokai Establishment,
Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan

AND

TSUNEO AMANO

Plasama Physics Laboratory, Faculty of Engineering,
Osaka University, Suita, Osaka, Japan

Received October 18, 1976; revised February 1, 1977

Diffusion equations of impurities with ionization and recombination source terms are solved numerically by the splitting and fractional-step method for noncommutative operators. Diffusion equations without source terms and rate equations are solved successively and the very small time step for calculation determined by fast ionization processes can be avoided by solving the rate equation as an eigenvalue problem. The time step is determined by the diffusion process and it is possible to follow the time evolution of impurities for a long time. The present method is second-order accurate in Δt.

1. INTRODUCTION

Small amounts of impurity ions emitted from the wall and limiter play an important role in thermonuclear devices such as Tokamaks. It is well known that impurities enhance the radiation losses of a plasma and have a tendency to accumulate in the center of plasma [1] so that they have a serious effect on the plasma confinement and heating. However, impurity behavior is a complicated process which includes an atomic process of ionization and recombination as well as a diffusion process. (See Eq. (1).)

The present paper is devoted to a new method for solving the diffusion equation of impurities such as carbon, oxygen, iron, molybdenum, etc. The solution of imputriy diffusion equations is a difficult numerical problem. Ionization and recombination terms contain various characteristic times which depend strongly on the electron temperature and vary on a wide range. Some of the characteristic times become comparable with those of diffusion. Therefore the diffusion and atomic terms should be treated simultaneously and the time step required for computation must be chosen to be smaller than the fastest ionization characteristic time which is much smaller

0021-9991/78/0261–0080$02.00/0

than that of diffusion. Previous work on impurity behavior in Tokamaks has been based on the diffusion equation for impurities [2, 3]. However, it seems that these methods for solving the equation have not yet been satisfactory for treating the diffusion and atomic processes simultaneously and consistently.

The present numerical technique employs a splitting and fractional-step method for noncommutative operators [4, 5]. The impurity diffusion equation is split into two kinds of equations—a diffusion equation without source terms and a rate equation. The diffusion equation is solved by the usual methods such as the Crank–Nicholson scheme and the recurrence relation [6]. The rate equation, which is linear, is treated as an eigenvalue problem in order to remove the very small time step restricted by fast ionization processes. It is possible to follow the impurity evolution by a larger time step Δt which can be determined by the diffusion characteristic time. The present method is indeed second-order accurate in Δt.

2. Numerical Method

In the present section, we consider the diffusion equation given as follows:

$$\frac{\partial n_k}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_k) + n_e(\alpha_{k-1}n_{k-1} - \alpha_k n_k) - n_e(\beta_{k-1}n_k - \beta_k n_{k+1}),$$
$$k = 1, 2,\ldots, K, \quad \alpha_0 = \beta_0 = \alpha_K = \beta_K = 0, \tag{1}$$

where n_k is number density of the imputiry ions with $(k - 1)$ electric charge (s), Γ_k is the particle flux of impurities with k, n_e is the electron density, and α_k and β_k are the rate coefficients for ionization from state k to state $k + 1$ and for recombination from state $k + 1$ to state k. These rate coefficients depend strongly on the electron temperature, T_e, which varies widely over space. In this section, we assume the linear form of Γ_k, for which concrete expressions are omitted here. The spatial difference equation for Eq. (1) has the form of

$$d\mathbf{u}/dt = A\mathbf{u} + B\mathbf{u} + \mathbf{a}, \tag{2}$$

with the boundary condition $\partial n_k/\partial r = 0$ at $r = 0$. In Eq. (2), $\mathbf{u}$ is the vector consisting of $(n_k)_j$'s, where $k = 1, 2,\ldots, K$ and $j = 2, 3,\ldots, J - 1$, and $\mathbf{a}$ is a vector consisting of $(n_k)_J$'s which are boundary values at the outermost mesh point J. A and B are matrices representing the diffusion term and the atomic process, respectively. The explicit expressions of A, B, and $\mathbf{a}$ are not given here since they are not necessary for the discussion below. It should be noted that A and B do not commute because n_e depends on r, and α_k and β_k depend strongly on T_e.

We assume that A, B, and $\mathbf{a}$ are constant in time during a small time step Δt and that $\mathbf{u}_0 = \mathbf{u}\ (t = 0)$ is known. The solution to Eq. (2) after Δt is

$$\mathbf{u}(\Delta t) = e^{(A+B)\Delta t}\{\mathbf{u}_0 + (A + B)^{-1}\mathbf{a}\} - (A + B)^{-1}\mathbf{a}. \tag{3}$$

We consider the approximation of Eq. (3) as follows:

$$\mathbf{u}(\Delta t) = e^{\frac{1}{2}B\Delta t}\{e^{A\Delta t}(e^{\frac{1}{2}B\Delta t}\,\mathbf{u}_0 + A^{-1}\mathbf{a}) - A^{-1}\mathbf{a}\}. \tag{4}$$

By Taylor expansions, we know that Eq. (4) approximates Eq. (3), with an error that is third order in Δt. According to Eq. (4), we can obtain solutions successively as follows:

First step. Solve the rate equations:

$$dn_k/dt = n_e(\alpha_{k-1}n_{k-1} - \alpha_k n_k) - n_e(\beta_{k-1}n_k - \beta_k n_{k+1}), \qquad k = 1, 2,..., K, \tag{5}$$

on all mesh points under the initial condition $\mathbf{u}_0$. The solutions to Eq. (5) at time $\Delta t/2$ give $\mathbf{u}_1 = e^{\frac{1}{2}B\Delta t}\mathbf{u}_0$. Because $\mathbf{u}_1$ is the solution at $\Delta t/2$ of

$$d\mathbf{u}/dt = B\mathbf{u}, \tag{6}$$

solving Eq. (6) corresponds to solving rate equations on all mesh points since Eq. (5) contains no spatial differentiation.

Second step. Solve the diffusion equations without source terms:

$$\frac{\partial n_k}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_k), \qquad k = 1, 2,..., K, \tag{7}$$

under the initial condition $\mathbf{u}_1$. The solutions to Eq. (7) at time Δt give $\mathbf{u}_2 = e^{A\Delta t}(\mathbf{u}_1 + A^{-1}\mathbf{a}) - A^{-1}\mathbf{a}$. Because $\mathbf{u}_2$ is the solution at Δt of

$$d\mathbf{u}/dt = A\mathbf{u} + \mathbf{a}, \tag{8}$$

solving Eq. (8) corresponds to solving the diffusion equation since Eq. (8) is the difference form of Eq. (7).

Third step. Solve the rate equations on all mesh points under the initial condition $\mathbf{u}_2$. The solutions at time $\Delta t/2$ give $\mathbf{u}_3 = e^{\frac{1}{2}B\Delta t}\mathbf{u}_2$. Then, $\mathbf{u}_3$ is the approximate solution to Eq. (1) of second-order accuracy in Δt.

Thus, one can replace a complicated problem given by Eq. (1) by a succession of simpler ones—diffusion equations and rate equations. This corresponds to the splitting and fractional-step method for noncommutative operators which has been suggested by Knorr [5]. Actually, the diffusion equation at the second step is solved numerically by, say, a Crank–Nicholson scheme and a recurrence relation [6]. On the other hand, the rate equation at the first and third steps should be solved so as to remove very short time step determined by the ionization process. We treat the rate equation as an eigenvalue problem. This method avoids the computational time step and furthermore has a merit that we do not need to solve the eigenvalue equation of Eq. (5) again at the third step once we obtain the eigenvalues and eigenvectors at the first step which are held constant during Δt.

Another form of Eq. (3) by the splitting and fractional-step method is given by

$$\mathbf{u}(\Delta t) = e^{\frac{1}{2}A\Delta t}[e^{B\Delta t}\{e^{\frac{1}{2}A\Delta t}(\mathbf{u}_0 + A^{-1}\mathbf{a}) - A^{-1}\mathbf{a}\} + A^{-1}\mathbf{a}] - A^{-1}\mathbf{a}, \tag{9}$$

which produces the approximation to Eq. (3) of second-order accuracy in Δt again. The algorithm in this case is as follows. First, solve diffusion equation (7) under the initial condition $\mathbf{u}_0$ and obtain solutions at time $\Delta t/2$; second, solve rate equations (5) on all mesh points under the initial condition of the first step solution and obtain solutions at time Δt; and third, solve the diffusion equation again and obtain solutions at time $\Delta t/2$ under the initial condition of the second solutions.

The former case based on Eq. (4) requires solving the diffusion equation once and the eigenvalue equation once on every mesh point, while the latter based on Eq. (9) needs to solve the diffusion equation twice as well as to solve the eigenvalue equation once on every mesh point. However, the former must store eigenvalues and eigenvectors on each mesh point, which requires a large memory if we treat heavy elements such as molybdenum ($Z = 42$) or tungsten ($Z = 74$).

3. Numerical Example

In this section we present a numerical example. The purpose of this section is not to investigate impurity behavior in a Tokamak plasma in detail but to test the new method described in the preceding section; therefore we restrict ourselves to the simplest case for particle flux and rate coefficients. In the Pfirsch–Schlüter regime in a Tokamak plasma, the simplest form for particle flux has the form [7]

$$\Gamma_k = -D_k \frac{\partial n_k}{\partial r} + D_k \frac{k-1}{Z_i} \frac{1}{n_i} \frac{\partial n_i}{\partial r} n_k, \tag{10}$$

$$D_k = (1 + 2q^2) \frac{4(2\pi m_i)^{1/2} c^2 Z_i^2 e^2 n_i \ln \Lambda}{3T_i^{1/2} B_0^2}, \tag{11}$$

where Z_i, n_i, m_i, and T_i are electric charge number, density, mass, and temperature of the plasma ions, respectively; Λ is the Coulomb logarithm; B_0 is the magnetic field strength; and q is the safety factor. The second term of Eq. (10) represents the diffusion due to frictional force between plasma and impurity ions which causes impurities to diffuse toward the center of the plasma [1]. It is difficult to estimate rate coefficients α_k and β_k precisely. Here we employ the rough estimation given by Hinnov [8], the forms of which are abbreviated in the present paper.

We have adopted the simplest form for Γ_k, α_k, and β_k in order to check the present method. However, if we intend to use the present method for the sake of the precise investigation of impurity behavior and its effect on a Tokamak plasma, we should consider a more precise and general form for particle flux [9] and the dielectronic recombination [10] should be taken into account. Further, in general, we should solve the impurity diffusion equation (1) simultaneously with particle and energy balance equations for plasma ions and electrons when we investigate the one-dimensional behavior of impurities in a Tokamak plasma. However, for simplicity, we restrict ourselves to the case when plasma profiles remain constant in time throughout the computation. The extension to the general case can be easily achieved.

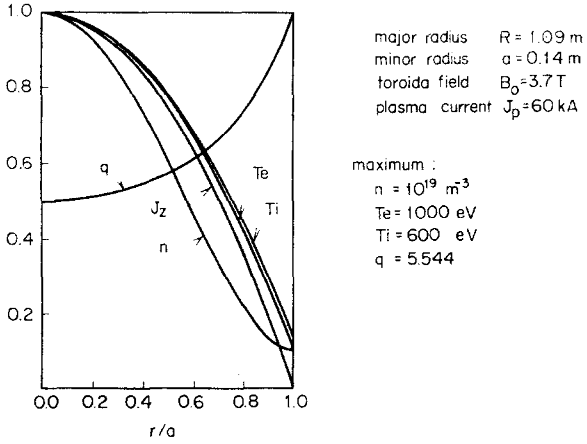


FIG. 1. Plasma distributions fixed throughout the computation.

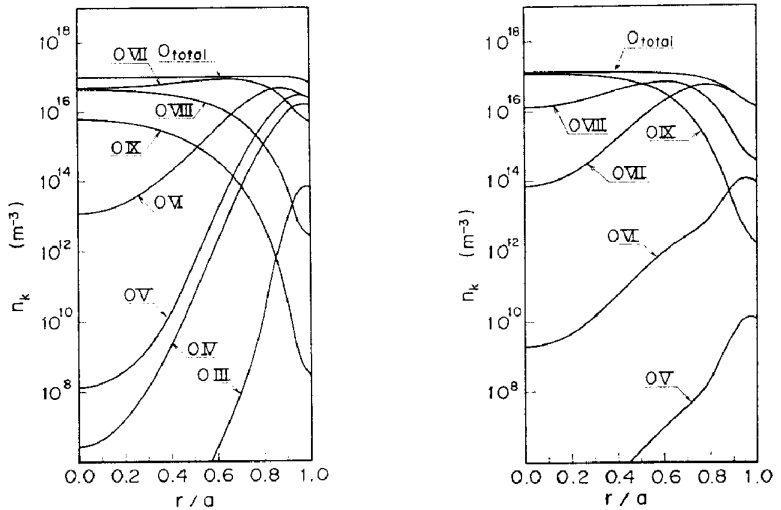
The time development of the profiles of oxygen impurties was followed by the method based on Eq. (4) assuming the constant plasma distributions shown in Fig. 1. Rate equations were solved as eigenvalue problems (the method is referred to in [11]), and diffusion equations were solved by a Cranck–Nicholson scheme. For an initial condition, we have distributed neutral oxygen with density of 10^{17} m^{-3} uniformly over the space. Boundary values were chosen so as to keep the total impurity density constant inside the plasma;

$$\frac{\partial}{\partial t}\int_0^a \sum_k n_k r\, dr = -a\sum_k \Gamma_k(r = a) = 0. \tag{12}$$

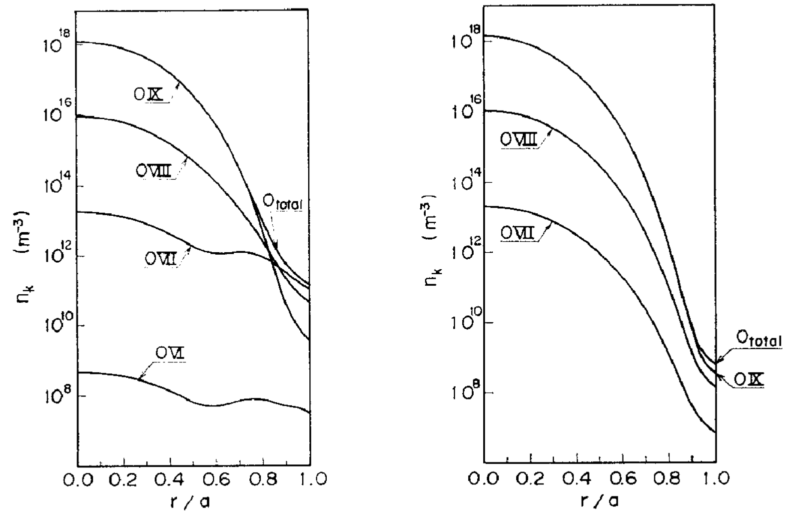
With this condition, steady-state distributions of impurities are easily obtained. To satisfy Eq. (12), we set $\Gamma_k = 0$ for all k, for simplicity. These initial and boundary conditions have no physical basis, since, in reality, they are very complicated because of plasma–wall interactions such as recycling and sputtering phenomena. The total number density of impurities was checked for computational validity. Relative errors of Eq. (12) were below 10^{-3} for $\Delta t = 10^{-4}$ sec and space mesh points of 25. Figure 2 shows the time development of the distributions of oxygen impurities. The steady-state solution was achieved after $t = 3.75 \times 10^{-1}$ sec in the present case. It is seen that impurities accumulate, as they are ionized successively toward the plasma center with time.

Another method based on Eq. (9) was compared with that of Eq. (4) under the same conditions as in Fig. 2. A fairly good agreement was obtained: The two have given the same result to an accuracy of five figures when the number of spatial mesh points was 50.

Finally, we have measured *cpu*-time for solving a rate equation once. The eigenvalue method required about 25, 40, and 320 msec for carbon ($K = 7$), oxygen ($K = 9$), and iron ($K = 27$), respectively. The *cpu*-time of the Runge–Kutta method



(a) $t = 10^{-3}$ sec (b) $t = 10^{-2}$ sec



(c) $t = 0.1$ sec (d) steady state

FIG. 2. Time development of the densities of oxygen impurities. At initial time oxygen with density of $10^{17}\ m^{-3}$ is distributed uniformly over the space: (a) $t = 10^{-3}$ sec, (b) $t = 10^{-2}$ sec, (c) $t = 0.1$ sec and (d) steady state.

depends strongly on the time mesh interval chosen for the computation. Minimum values of the ionization characteristic time given by $1/n_e\alpha_k$ over k's, and electron temperatures are about 10^{-6} sec (for CI → CII, $T_e = 100$ eV), 7.5×10^{-7} sec (for OI → OII, $T_e = 100$ eV), and 6.5×10^{-7} sec (for FeI → FeII, $T_e = 70$ eV), respectively, when $n_e = 10^{19} m^{-3}$. If we choose a Δt of one quarter of the minimum characteristic time for ionization, we obtain 130, 200, and 630 msec for carbon, oxygen, and iron, respectively, in order to solve the rate equation during 10^{-4} sec. The fact should be emphasized that the minimum characteristic time becomes shorter as the plasma density increases, which significantly affects the choice of the time step required for the computation by the Runge–Kutta method. On the other hand, the eigenvalue method is completely free from the time mesh interval.

The present computations were performed by the electronic computer FACOM 230/75 at the data processing center in the Japan Atomic Energy Research Institute.

4. CONCLUSION

It is found that diffusion equations for impurity ions with source and sink terms due to ionization and recombination can be replaced by a succession of simpler ones. Solving rate equations and diffusion equations successively according to Eq. (4) or Eq. (9) gives approximate solutions of second-order accuracy in Δt. It has been proposed that the rate equation should be treated as an eigenvalue problem to remove the very small time step determined by ionization process. In general, diffusion equations are nonlinear when impurity–impurity collisions are not ignored. Such a case requires some numerical technique such as linearization or iteration. The method of solving impurity diffusion equations described in the present paper will be useful to investigate the time development of impurities in a Tokamak plasma using a one-dimensional Tokamak transport code.

REFERENCES

1. C. L. LONGMIRE AND M. N. ROSENBLUTH, *Phys. Rev.* **103** (1956), 507.
2. V. I. GERVIDS AND V. A. KRUPIN, *JETP Lett.* **18** (1973), 106.
3. D. M. MEADE, H. P. FURTH, P. H. RUTHERFORD, F. G. P. SEIDL, AND D. F. DÜCHS, *in* "Plasma Physics and Controlled Nuclear Fusion Research 1974" (Proc. 5th Int. Conf. Tokyo, 1974, IAEA-CN-33/A15-4), Vol. I, p. 605.
4. R. D. RICHTMYER AND K. W. MORTON, "Difference Methods for Initial-Value Problems" (R. D. Richtmyer, Ed.), 2nd ed., p. 216, Wiley–Interscience, New York, 1967.
5. G. KNORR, *in* "Proceedings of the 2nd European Conference on Computational Physics" (D. Biskamp, Ed.), Session D.3, 1976.
6. R. D. RICHMYER AND K. W. MORTON, *in* "Difference Methods for Initial-Value Problems," (R. D. Richtmyer, Ed.), 2nd ed., p. 198, Wiley–Interscience, New York, 1967.
7. T. TUDA AND M. TANAKA, *J. Phys. Soc. Japan* **38** (1975), 1228.
8. E. HINNOV, Matt-777, Princeton Plasma Physics Laboratory, Princeton University, 1970.
9. For example, F. L. HINTON AND T. B. MOORE, *Nucl. Fusion* **14** (1974), 639; P. ROLLAND AND J. REND, *in* "Plasma Physics and Controlled Nuclear Fusion Research" (Proc. 6th Int. Conf. Berchtesgaden, 1976, IAEA-CN-35/B-8-3).
10. A. BURGESS, *Astrophys. J.* **139** (1964), 776; **141** (1965), 1588.
11. T. AMANO AND M. OKAMOTO, JAERI-M 6401, Japan Atomic Energy Research Institute, 1976.