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Algorithms for the Calculation of Ionization in Rapidly Changing Plasmas

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Two simple algoriths are presented, suitable for the determination of ionization in plasmas with rapidly changing thermodynamic state, such as produced by laser irradiation of solid targets. The algorithms are designed to run with a large time step and yet be stable and reasonably accurate.

INTRODUCTION

The numerical modeling of plasmas using multicelled hydrodynamical techniques is by now well established. In general these numerical plasmas incorporate an appropriate equation of state for the plasma conditions under study. Such equations of state are usually calculated under steady state equilibrium conditions, and then applied to a time varying hydrodynamic system. In many cases this does not lead to error, as relaxation times are frequently faster than the other time scales in the problem. This may not, however, be true of ionization phenomena, which often tend to be slow. Indeed under conditions of frozen ionization [1] we may actually seek to study the development of plasma in this nonequilibrium state. For this purpose it is desirable to have suitable algorithms for calculating ionization which use a minimum of computer mill-time and have minimal storage requirements, and can be included within a multicell hydrodynamics code.

The simultaneous integration of the ionization rate equations with the equations of hydrodynamics introduces several complicating factors, particularly if a fluid cell technique is used. Considerations of computer storage dictate that only one time level be stored, so that neither Runge–Kutta nor predictor–corrector techniques can be used. Since the various rates are generally given by complicated analytic forms, these should clearly be calculated as infrequently as possible, i.e., on the hydrodynamic time scale. Under conditions of high density the ionization time scale may be much shorter than the hydrodynamic one, so that the ionization must be integrated separately from the hydrodynamics. A simple method of doing this, by integrating the ionization several times with a small time step within the hydrodynamic step, is satisfactory, but slow. A better alternative is to integrate with an algorithm which allows the use of the hydrodynamic time step directly. However, stability considerations influence the choice of such integration schemes. The ionization rate equation is similar in form to the spatial finite difference form of the diffusion equation which is well known to

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have stability problems in an explicit form; so that an implicit scheme should be used. We have found that such an implicit form modified by an appropriate weighting factor can be used satisfactorily at the large hydrodynamic time step; the weighting factor being determined by comparison with an analytic solution. We have also found satisfactory a second algorithm—the two-stage scheme—which is based on a quasi-analytic solution of the rate equations for large time steps. These algorithms may be used for any process such as ionization which exponentially approaches a final value. It is required that the algorithm be accurate to second order for small step lengths and converge iteratively for large ones. Due to the exponential nature of the process, the algorithms give a satisfactory description over the whole range of step lengths, with sufficient numerical accuracy and unconditional stability.

The ionization rate equations are a typical example of the general class of stiff equations [2]. Some standard methods for the numerical integration of these equations are well known [2]. However, since these have either large memory requirements (predictor–corrector schemes) or are slow (eigenvalue schemes) we have not considered them for the present application. For straightforward solution of the ionization rate equations these methods have several advantages over those described in this paper. The algorithms described here should not be regarded as alternatives to those discussed by Gear [2] but rather ones designed especially for inclusion in multicelled fluid codes.

The ionization and recombination rates must include multistep processes and a full analysis involves a complete description of each ionization stage with all its levels of excitation. The various processes may then be computed via a time dependent collisional radiative model [3]. Since this involves the calculation and integration of each interstate transition for each ionization stage, it is clearly a lengthy process, demanding of computer time. In this paper we assume the use of the averaged rate coefficients for each stage such as those derived from the collision limit approximation [4]. As a result the accuracy of the various rate equations cannot be expected to be great and the accuracy demanded of the calculations is therefore not high. However, we must be careful that in relaxing the conditions of accuracy we do not allow the computational procedures to become unstable.

THE IONIZATION RATE EQUATIONS

The development of ionization in a plasma is described by the ionization rate equations, which give the relative ionic populations. Thus the relative population, q_i, of the ith stage of ionization in a Lagrangian system is given by:

$$\frac{dq_i}{dt} = \mathscr{R}_{i+1} q_{i+1} - (\mathscr{R}_i + \mathscr{S}_i)_q + \mathscr{S}_{i-1} q_{i-1} \tag{1}$$

where $\mathscr{R}_i$ and $\mathscr{S}_i$ are the total recombination and ionization rates for the state i, respectively. These depend on the electron density in the following simple way:

$$\mathscr{S}_i = S_i n_e, \qquad \mathscr{R}_i = R_{1i} n_e + R_{2i} n_e^2, \tag{2}$$

where S_i is the ionization rate coefficient and R_{1i} and R_{2i} are the two- and three-body recombination rate coefficients, respectively. In general S_i, R_{1i}, and R_{2i} depend on the electron temperature but vary only weakly with the other plasma conditions, such as the electron density.

We can reduce the number of equations to be solved by introducing the ionization change across a step Δ_i

$$\Delta_i = q_i - q_i^0 + \Delta_{i-1}, \qquad \Delta_0 = 0, \tag{3}$$

where the q_i^0's are the values of q_i at some arbitrary time, usually considered to be the start of a time step. In terms of these variables (1) can be written

$$\begin{aligned} \frac{d\Delta_i}{dt} &= \mathscr{R}_{i+1} q_{i+1}^0 - \mathscr{S}_i q_i^0 \\ &\quad + \mathscr{R}_{i+1}\Delta_{i+1} - (\mathscr{R}_{i+1} + \mathscr{S}_i)\,\Delta_i + \mathscr{S}_i \Delta_{i-1}. \end{aligned} \tag{4}$$

IMPLICIT METHODS

The ionization rate equations (1) are simply an example of a restricted class of the more general family of rate equations. As is well known the solution of this type of problem leads to stiff equations for which standard methods are available. In general these are implicit multistep techniques, with a Newton iteration to the corrector [2]. However, as discussed earlier, computer storage requirements limit any scheme to only two steps, i.e., the trapezoidal method, the simple form of which can lead to spurious oscillation [5]. We have therefore sought to use a modified trapezoidal method for the ionization problem. In particular the tridiagonal nature of the equations allow great simplification in the solution of the implicit equations.

If we consider the electron density constant during the time step and write Eq. (4) in an implicit finite difference form with a variable weight factor, W_i :

$$\Delta_i - (1 - W_i)\{\mathscr{R}_{i+1}\Delta_{i+1} - (\mathscr{R}_{i+1} + \mathscr{S}_i)\,\Delta_i + \mathscr{S}_i\Delta_{i-1}\}\,\Delta t = \{\mathscr{R}_{i+1} q_{i+1}^n - \mathscr{S}_i q_i^n\}\,\Delta t \tag{5}$$

where values after n time steps are denoted by the superscript n. These equations are identical to those used in calculations of the diffusion equation and may be solved by the same well-known algorithm [6]. Since such implicit schemes are stable if the weights W_i satisfy $0 \leqslant W_i \leqslant 0.5$, our choice of the weight function is determined by the condition for stability, and that for large rates the solution to Eq. (5) exactly match the analytic solution if $\Delta_{i+1} = \Delta_{i-1} \simeq 0$. Thus:

$$W_i = \mathrm{Min} \begin{Bmatrix} 0.5 \\ 1/C_i - \exp(-C_i) \end{Bmatrix} \tag{6}$$

where $C_i = (\mathscr{R}_{i+1} + \mathscr{S}_i)\,\Delta t$. We have found in practice that the use of this simple weighting function allows a considerable gain in accuracy at large rates ($C_i \gg 1$), and in particular allows the ionization step $i \rightarrow i + 1$ to equilibrate properly.

The rates $\mathscr{R}_{i+1}$ and $\mathscr{S}_i$ both depend on the electron density, which in turn is a function of the fractional ionization; indeed the effective charge of the ions $Z\,(= n_e/n_i)$ is given by:

$$Z^{n+1} = Z^n + \sum_i \Delta_i \qquad (7)$$

where n_i is the total ion density. As a result with a poorly chosen step length and initial conditions far from equilibrium, delays and overshoot can occur as shown in Fig. 1. In practice this difficulty can be overcome by a simple iteration of the electron density (Fig. 1). In performing this iteration we have found it beneficial to calculate the electron density for use in determining $\mathscr{R}_i$ and $\mathscr{S}_i$ consistently with Eq. (5). Thus we use:

$$\tilde{n}_e = n_e^n + n_i^n \sum \Delta_i(1 - W_i). \qquad (8)$$

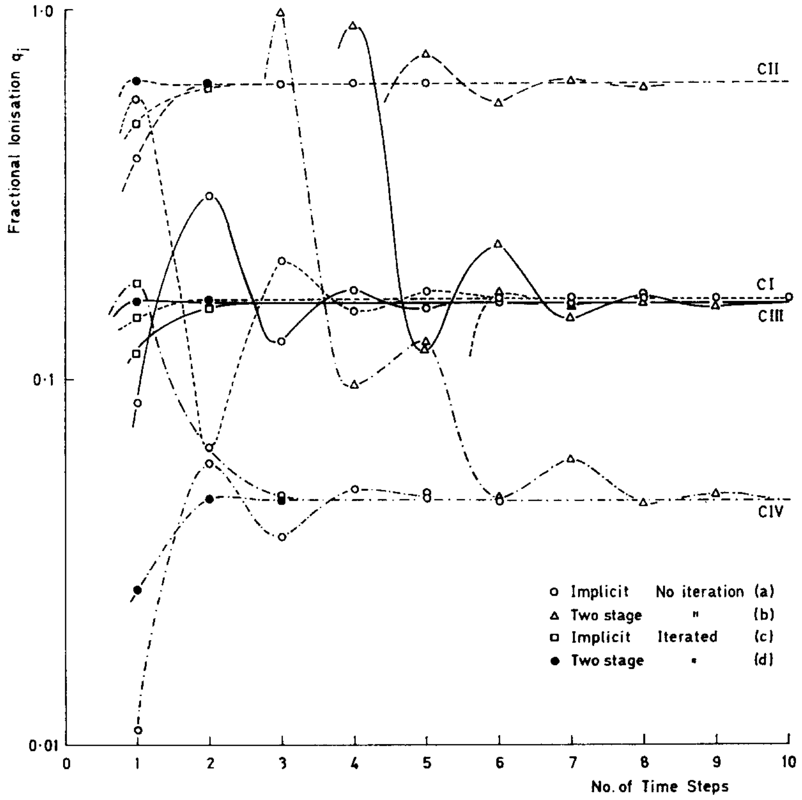

FIG. 1. Comparison of results using the various algorithms with and without iteration. A strongly recombining plasma is shown: in this case carbon initially fully stripped at a temperature of 10 eV and density $10^{22}/\text{cm}^3$. The time step chosen, 2.5 psec, was ridiculously large to demonstrate the limitations of the noniterated implicit and two-stage schemes. The first 10 time steps are shown.

A further improvement is obtained by linearizing Eq. (5) incorporating this term and including the terms in Δ_{i-1}, Δ_i, and Δ_{i+1} directly in the implicit scheme. It can be clearly seen from Fig. 1 that this modification overcomes the problems associated with poorly chosen initial conditions. In general we have found that no more than one such iteration is required in a practical case. We may note that this iterated algorithm is the second order form of the general class described by Gear [2], if Newton iteration is used for the complete set Δ_j; this, however, involves a considerably more complex matrix inversion than the scheme proposed here.

TWO STAGE SCHEME

A useful analytic form which leads to a stable computational scheme is obtained by integrating the rate equation (4) for each stage independently of the others. Thus we consider:

$$d\Delta_i/dt = (S_i q_i - R_{i+1} q_{i+1})\, n_e \tag{9}$$

and using Eq. (7) we obtain:

$$\Delta_i = \frac{ZB_i(1 - D_i)}{(Z + B_i D_i)} \tag{10}$$

where

$$B_i = (S_i q_i^n - R_{i+1} q_{i+1}^n)/(S_i + R_{i+1}) \tag{11}$$

and

$$D_i = \exp\{-(Z + B_i)(S_i + R_{i+1})\, n_i \Delta t\}. \tag{12}$$

The algorithm is obtained by progressively calculating the set Δ_i from (10) for each stage of ionization. The new values of q_i are then obtained recursively from the equations (2). A crude stability analysis (Appendix) shows that this algorithm is stable for all decaying solutions and relatively stable for growing ones.

This algorithm, while not as accurate as the previous one, has the advantage that each ionization stage is treated separately allowing a different treatment for specific stages if desired: in fact, the algorithm was developed to use with a complete collisional-radiative description of specified ionization stages, which can thus each be treated separately with a consequent saving in computer time. The two stage scheme has proved very successful in practice and is more accurate than might at first be expected. The reason for this is that the processes of ionization and recombination are such that in practice one ionization step dominates at the expense of the others.

As with the implicit scheme this algorithm can also give rise to spurious delays and overshoot with badly chosen initial conditions (Fig. 1). In this case the problems are associated with the fact that changes can only take place across one ionization stage per time step. Although the initial errors are large we note that they are rapidly damped. These errors are also inhibited by iteration (Fig. 1).

When iterative methods are used, we have found that the accuracy can be improved by using weighted values to calculate Δ_i. Thus we write.

$$\tilde{Z}_i = Z^n + (1 - W_i) \sum_{i \neq j} \Delta_j$$

and

$$\begin{aligned} \tilde{q}_{i+1} &= q^n_{i+1} - (1 - W_i)\, \Delta_{i+1}\,, \\ \tilde{q}_i &= q_i^n + (1 - W_i)\, \Delta_{i-1} \end{aligned} \tag{13}$$

in Eqs. (10)–(12) in place of Z, q_{i+1}, and q_i, respectively. Clearly the weights W_i must satisfy $0 \leqslant W_i \leqslant 1$ by the mean value theorem. In fact. for small rates ($D_i \to 1$) $W_i = \frac{1}{2}$ gives second order accuracy. For large values of the rates ($D_i \to 0$) the solution iterates to the steady state if $W_i = 0$. A suitable value with these properties which in addition reduces to the exact three stage solution in the limit $Z \gg | B_i |$ is:

$$W_i = \mathrm{Min}\,(0.5, D_i) \tag{14}$$

which has proved satisfactory. In practice it is unlikely that one would use repeated iteration of this method, although a single iteration may be useful on occasion. If repeated iteration is used it can be shown that the iteration will converge. Either direct substitution or Newton's method can be used; but the fastest method is obtained by using Newton's method for the tridiagonal terms and direct substitution for the others, as one may then use the rapid tridiagonal matrix inversion procedure [6].

THE ENERGY LIMIT

The step length, Δt, is chosen so that any variations due to the expansion are relatively small during each interval. Thus n_i is approximately constant during the integration of (1) and in the two stage scheme variation of n_e is taken into acount by Eqs. (8) and (12). However, due to the energy required for ionization, the electron temperature may vary significantly over an integration step, causing a significant change in the appropriate rates when the ionization energy is included in the total electron energy balance. At large rates when the system is near equilibrium this may lead to an oscillation.

Assume that at each ionization calculation the system equilibrates and consider an iteration for the temperature deviation ΔT_e. The change in ionization at each iteration:

$$\Delta q_i \simeq (dq_i/dT_e)\, \Delta T_e \tag{15}$$

and the next iteration of $\Delta T_e'$ is given by an energy balance:

$$\begin{aligned} \tfrac{3}{2} Zk\Delta T_e' &\simeq - \sum (\tfrac{3}{2}kT_e + V_i)\, \Delta q_i \\ &= - \sum (\tfrac{3}{2}kT_e + V_i)(dq_i/dT_e)\, \Delta T_e \end{aligned} \tag{16}$$

where Z is the average ionic change.

Thus if $|\sum(\frac{3}{2}kT_e + V_i)(dq_i/dT_e)| > \frac{3}{2}Zk$ the iteration will grow unstably. In a similar manner these iterations occur in the usual calculations and lead to a similar unstable growth. To prevent this oscillation growth we have introduced an "energy limit," whose effect is to limit the amount of energy transfer which can occur in a given calculation step.

If an incremental temperature rise $\Delta T_e'$ is calculated without the inclusion of the ionization changes the true incremental rise ΔT_e is given by:

$$\tfrac{3}{2}Zk\Delta T_e \simeq -\sum_i(\tfrac{3}{2}kT_e + V_i)\,\Delta q_i + \tfrac{3}{2}Zk\Delta T_e'. \tag{17}$$

Calculation of the fractional ionization change with increments $\Delta T_e'$ and ΔT_e yields $\Delta q_i'$ and Δq_i, respectively, given by (15). Thus

$$\Delta q_i \simeq \Delta q_i' \Big/ \Big(1 + \sum(\tfrac{3}{2}kT_e + V_i)\,\Delta q_i' \Big/ \tfrac{3}{2}Zk\Delta T_e'\Big). \tag{18}$$

Since $(\frac{3}{2}kT_e + V_i)\,\Delta q_i'$ is the heat exchange in ionization, we may regard Eq. (18) as specifying a limiting heat exchange $\frac{3}{2}Zk\Delta T_e'$; namely, that associated with the temperature change $\Delta T_e'$, to prevent oscillation. In fact we may note that Eq. (18) is equivalent to a Newton–Raphson iteration term.

In cases far from equilibrium some form of physical energy limit will apply (although it is unlikely to be particularly important under these conditions), due to the rapid variation of ionization rate with temperature. This will limit the energy transfer to some value

$$\Delta E \sim \tfrac{3}{2}Zk(\Delta T_e' + \alpha T_e) \tag{19}$$

where $\alpha \sim 0.5$.

In practice to treat this situation generally we have found a suitable form for α to be given by:

$$\begin{aligned} &\alpha = 0.5\sum \beta_i(q_i + q_{i-1})/\sum(q_i + q_{i-1}),\\ &\beta_i = \text{if } \Delta < 0.9 \text{ then } (1.0 - \exp[-(q_i - q_i^0)^2/q_i q_i^0])/2 \text{ else } 1.0 \end{aligned} \tag{20}$$

where for the implicit method Δ is given by $\exp(-C)$ with C given by (6) and by (12) for the two-stage method.

It should be noted that this instability only arises if there is an energy exchange between ionization and the electron temperature: in fact Eqs. (16) and (17) assumed a complete exchange. Clearly if the plasma is recombining radiatively and is optically thin this assumption does not apply. However, in laser plasmas this situation only occurs when the ionization processes are slow and the energy limit, given by (19), places no restriction on the ionization change.

It is clear from the nature of the energy limit that we must estimate the electron energy balance including all other terms, such as ion–electron equilibration, thermal conduction, radiation transfer, etc. This is most conveniently done by calculating these in the absence of ionization before treating the ionization last within a split time step scheme. If an equilibration scheme [7] is used for terms such as ion–electron transfer, some error in electron temperature may be incurred thereby, but the energy limit itself ensures that it does not exceed $\Delta T_e'$, which is presumably limited by other constraints within the program to be small.

In Fig, 2 the behavior of the electron temperature in a typical computational run is shown with and without the various energy limit terms. It can be clearly seen that only when the complete energy limit given by Ed. (20) is used is this instability eliminated. This result has been confirmed by subsequent satisfactory experience with this term.

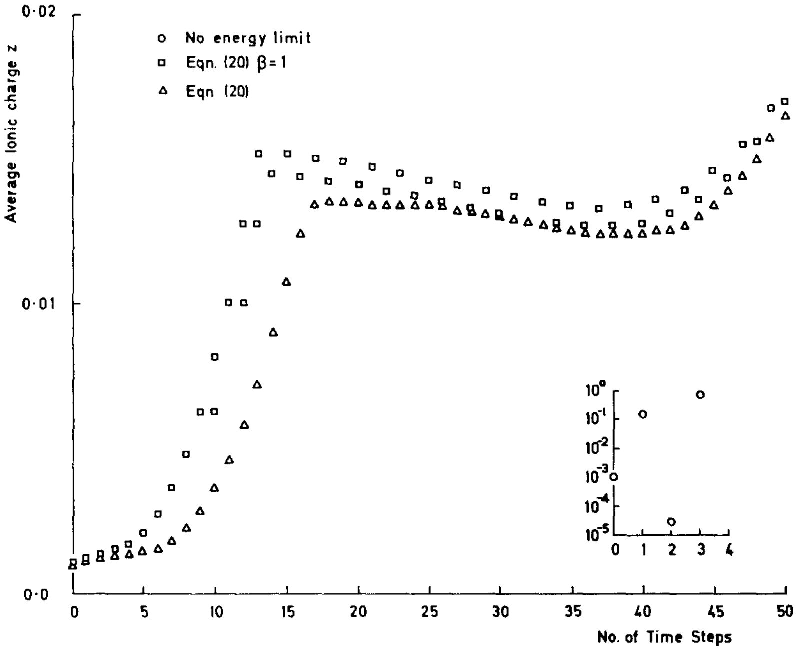

FIG. 2. Demonstration of the effect of the energy limit. The plasma was an initially unionized carbon fiber heated by 100-*GW* laser pulse. It can be seen that with no energy limit a catastrophic oscillation occurred very rapidly. With $\beta = 1$ in Eq. (20) some oscillation occurred, which became stronger later in the program. Only with β given (20) is this oscillation prevented.

The small inset diagram in Fig. 2 shows the behavior with no energy limit at all. It can be clearly seen that the integration rapidly becomes unstable and after four time steps causes overflow within the program. The inclusion of a simple energy limit given by Eq. (20) with $\beta = 1$ prevents this catastrophic instability, but some overshoot and subsequent oscillation occurs. With the value of β given in (20) the rise of ionization is not inhibited and little overshoot and no oscillation occurs. This solution subsequently remained stable throughout the course of integration, whereas that with $\beta = 1$ subsequently developed a substantial oscillation.

DISCUSSION AND CONCLUSIONS

The algorithms described in the previous sections have been regularly used in a number of programs to investigate the ionization development of laser-produced plasmas. In general the implicit algorithm has been used in cases where the average charge state and the ionic populations only are required, and the two-stage scheme in conjunction with a detailed atomic physics subroutine to study the excited state population levels in various ionization stages. Both algorithms have been incorporated into a standard one-dimensional Lagrangian code to model the laser plasma hydrodynamics: Lagrangian codes are particularly suitable for this application as there is no advection term involving the transfer of ionization between cells. In addition the two-stage algorithm is used with the atomic physics package in an averaged self-similar hydrodynamics code to study population inversion growth in recombining plasmas in connection with an *XUV* laser study. In Figs. 3. and 4 we show an example of each of the applications.

Figure 3 shows a typical example using the implicit scheme in the one-dimensional Lagrangian code. A *Nd* glass laser pulse of intensity 4 × 10^{21} W/cm^2 lasting

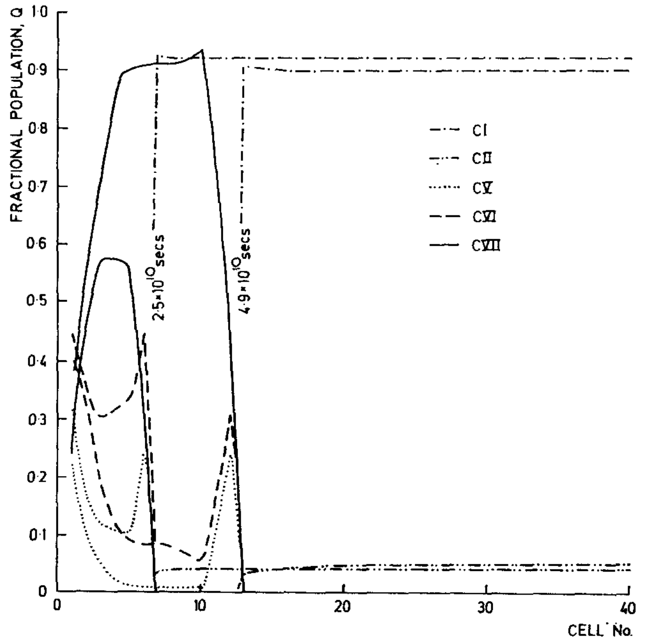

FIG. 3. Plots of the ionization in a typical laser–solid-target computation. A laser pulse of intensity 4 × 10^{21} *W*/cm^2 and duration 2.5 × 10^{-10} sec is incident on a solid carbon surface. The ionization fractions at times 2.5 × 10^{-10} and 4.9 × 10^{-10} sec after the initiation of the pulse are shown. It can be seen that only weak ionization (CI and CII) occurs behind the shock wave, but that strong ionization (CV, CVI, and CVII) is associated with the sharp thermal conduction front. The calculation was performed using a one-dimensional Lagrangian code with initial cell size 6.25 × 10^{-7} cm.

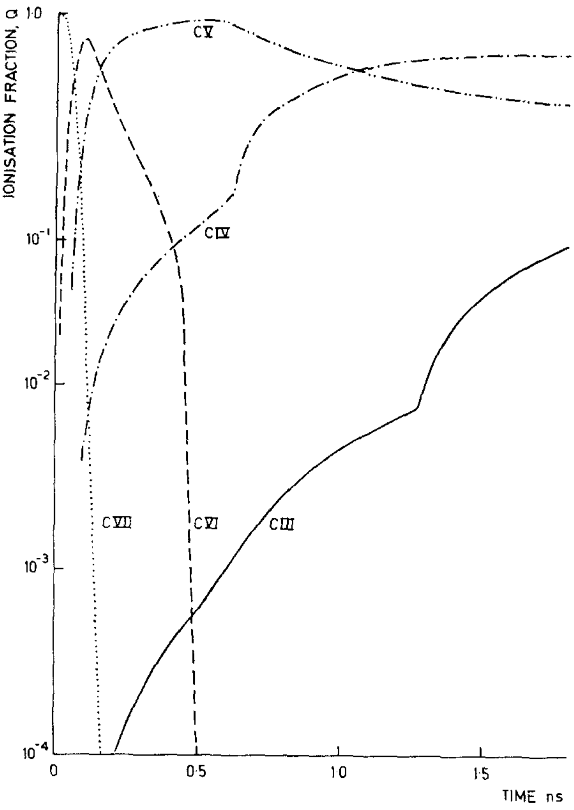

Fig. 4. Plots of the ionization and recombination following the absorption of 5 J of energy in a spot of 20-μm radius on a solid carbon surface. The initial effective charge, z, was 10^{-3}. The marked changes in the recombination rate at 0.4, 0.5, and 1.3 nsec are due to the use of the collision limit approximation for the rates.

2.5×10^{-10} sec is incident on a carbon slab: the Lagrangian cell size was 6.25×10^{-7} cm. This case is a fairly typical laser–solid-target interaction. A shock wave runs into the solid ahead of the thermal conduction front. Only weak ionization occurs associated with the shock, but in the conduction heated zone ionization is nearly complete. The ionization further increases in the expansion fan as the density decreases, but thermal conduction maintains the electron temperature, so that the Saha equilibrium ionization fractions increase. This example is typical of slab targets in that the ionization is practically equilibrated throughout, except in the extreme low density regions of the expansion fan. Thus in practice it is not usually necessary to use a time dependent code for these calculations. They do, however, give a good test of such a code, since as noted earlier it is in such regions that the energy limit instability occurs. Furthermore, the prevalance of such regions in these flows requires that the code properly equilibrate—a condition ensured in this case by the weights W_i. In this example the time step was limited by the Courant–Friedrichs–Levy condition on the hydrodynamics; a total of 15,000 time steps was used for this calculation.

Our second example uses the implicit scheme with the similarity model hydrodynamics to calculate the ionization in the expansion following the instantaneous deposition of 5 J of laser energy in a spot of 20-μm radius on a carbon slab. The Caruso–Salzmann [8, 9] theory is used to calculate the initial plasma condition. In contrast to the previous case, the ionization in this case is strongly time dependent, since the characteristic hydrodynamic time scale is of the same order or less than the ionization time. In the early stages of the calculation the plasma rapidly ionizes, before strong cooling due to expansion induces recombination. At later times the rapid decrease in electron density leads to the production of a state of frozen ionization. The calculation of the populations in this frozen state can only be accomplished by a time dependent calculation such as that used here. We note that this calculation is stable throughout.

We may briefly summarize our experience with these algorithms as follows:

(1) For most calculations noniterative routines are satisfactory.

(2) If the rates are described by the collision limit approximation (i.e., the populations of bound electronic states are not explicitly treated) the implicit method is best. The two-stage scheme is mainly used in conjunction with complete collisional–radiative calculations of designated ionization stages.

(3) One should always include the energy limit if steady state conditions are approached.

(4) In situations initially far from steady state where rapid equilibration is expected, one should try to adjust the initial time interval to ensure that the dominant ionization stage changes by only one per time step. Once the steady state is approached this condition can be relaxed.

(5) If noniterated schemes are used a considerable saving in time is obtained by only performing the calculations for ionization steps whose total population ($q_i + q_{i+1}$) is significant. However, note that such a procedure used with the implicit method may lead to delays and oscillations similar to the two step (Fig. 1) in cases of rapid ionization change.

APPENDIX: STABILITY OF THE TWO-STAGE ALGORITHM

To consider the stability of the two stage scheme it is convenient to consider the propagation of errors in the terms Δ_i. Thus if Δ_i^n is the value obtained in the nth time step:

$$q_i^n = q_i^0 + \sum_{j=1}^{n} (\Delta_{i-1}^j - \Delta_i^j) = \sum_{j=0}^{n} (\Delta_{i-1}^j - \Delta_i^j) + \delta_{i0} \qquad \text{(A.1)}$$

where δ_{ij} is the Kronecker delta, and the values Δ_i^0 are chosen to match the initial conditions.

Hence:

$$Z^n = Z^0 + \sum_{j=1}^{n} \sum_{i} \Delta_i^j = \sum_{j=0}^{n} \sum_{i} \Delta_i^j. \tag{A.2}$$

The errors are propagated by the amplification matrix G_{ij}

$$\Sigma_i^{n+1} = \sum G_{ij} \Sigma_j^n \tag{A.3}$$

where

$$\begin{aligned} G_{ii} &= (Z + B_i)^2 D_i/(Z + B_i D_i)^2, \\ G_{i,i\pm1} &= [B_i^2 D_i(1 - D_i) + Z^2(1 - D_i) \left\{ {\beta_i \atop \alpha_i} \right\} - Z B_i D_i \ln D_i (1 + \left\{ {\beta_i \atop \alpha_i} \right\})]/(Z + B_i D_i)^2, \\ G_{i,j} &= [B_i^2 D_i(1 - D_i) - Z B_i D_i \ln D_i]/(Z + B_i D_i)^2, \quad j \neq i, i + 1, i - 1, \end{aligned} \tag{A.4}$$

where

$$\alpha_i = R_{i+1}/(R_{i+1} + S_i) \text{ and } \beta_i = S_i/(R_{i+1} + S_i).$$

As is well known the condition for the stability of the algorithm is determined by the eigenvalues of the matrix G_{ij}. However, in view of the difficulty in calculating these for general values of Z, B_i, α_i, and β_i, we have found it necessary to adopt a simpler criterion for stability namely, that the matrix G must satisfy the conditions:

(i) The growth in any error term Σ_i due to a second Σ_j be less than unity, i.e.,

$$| \Sigma_i^{n+1} | \leqslant | \Sigma_j^n |, \qquad \text{i.e., } | G_{ij} | \leqslant 1 \tag{A.5}$$

for all values of i and j.

(ii) The variance of the errors must decrease

$$\sum_i (\Sigma_i^{n+1})^2 \leqslant \sum_i (\Sigma_i)^2. \tag{A.6}$$

Assuming the errors behave as though randomly distributed

$$\sum_i (\Sigma_i^n)^2 \geqslant \sum_{i,j} (G_{ij} \Sigma_j^n)^2. \tag{A.7}$$

This condition is satisfied if

$$\sum_i (G_{ij})^2 \leqslant 1 \qquad \text{for all } j. \tag{A.8}$$

A more convenient condition is obtained if all the errors have nearly the same value:

$$\sum_j (G_{ij})^2 \leqslant 1 \qquad \text{for all } i. \tag{A.9}$$

We consider the stability of the algorithm under the conditions (A5) and (A6). If these conditions are satisfied the algorithm is assumed to be absolutely stable. We may also consider the relative stability defined by the relative errors $\Sigma_i' = \Sigma_i/\Delta_i$. In common with most other workers we shall seek that the system be relatively stable for growing solutions and absolutely stable for decaying ones. As can be seen from Eq. (10) this implies:

$$\text{growing solution: } \Delta_i^{n+1} - \Delta_i^{n} > 0, \qquad B_i > 0, \qquad \text{relative stability;}$$

$$\text{decaying solution: } \Delta_i^{n+1} - \Delta_i^{n} < 0, \qquad B_i < 0, \qquad \text{absolute stability.}$$

The conditions (i) and (ii) may be similarly applied to relative stability and require that inequalities similar to (A5) and (A6) be satisfied for the matrix:

$$G'_{ij} = \frac{(Z + B_i D_i)}{(Z + B_i)} G_{ij} . \tag{A.10}$$

The Behavior of the Matrix G

We consider the functions:

$$\mathscr{F} = \frac{(1 + x)^2 D}{(x + D)^2} , \tag{A.11}$$

$$\mathscr{G} = \frac{(1 - D) D + x^2(1 - D) - 2xD \ln D}{(x + D)^2} , \tag{A.12}$$

$$\mathscr{H} = \frac{(1 - D) D - xD \ln D}{(x + D)^2} , \tag{A.13}$$

in the range $0 \leqslant D \leqslant 1$. The properties of these functions can be found in the usual way, but are most easily demonstrated graphically (Figs (A.1–A.3).

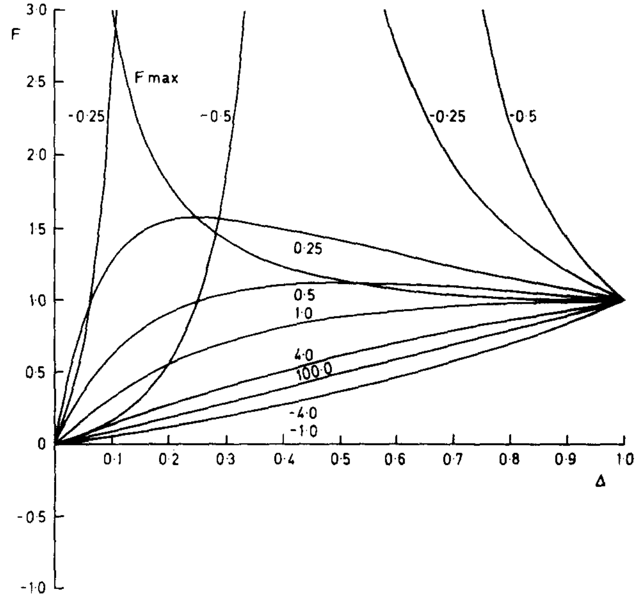

FIG. A1. Plot of the stability function $\mathscr{F}$ defined in Eq. (A11) in the range $0 \leqslant D \leqslant 1$ as a function of the parameter x. Also shown is the locus of the extrema of $\mathscr{F}$.

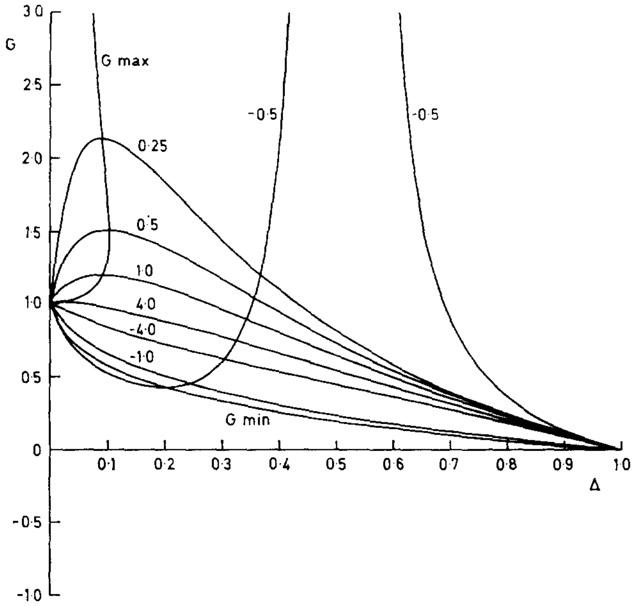

Fig. A2. Plot of the stability function $\mathscr{G}$ defined in Eq. (A12) in the range $0 \leqslant D \leqslant 1$ as a function of the parameter x. Also shown is the locus of the extrema of $\mathscr{G}$.

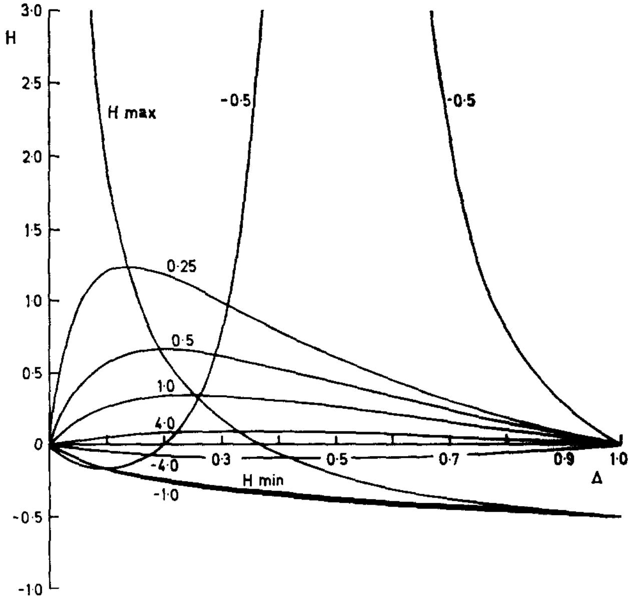

Fig. A3. Plot of the stability function $\mathscr{H}$ defined in Eq. (A13) in the range $0 \leqslant D \leqslant 1$ as a function of the parameter x. Also shown is the locus of the extrema of $\mathscr{H}$.

Hence since $0 \leqslant \alpha, \beta \leqslant 1$ we conclude that condition (i) is always satisfied, since the condition $Z \geqslant q_1$ limits the negative values of $x = Z/B_i$ to $-\infty \leqslant x \leqslant -1$. The condition (ii) cannot be so simply established. However, numerical evaluation for a wide range of values of q_i and x_i, β_i has shown this condition also to be always obeyed in practice.

A simpler analysis can be performed for the matrix G' with similar conclusions for the case $x \geqslant 0$.

We therefore conclude that the two-stage algorithm is:

(a) unconditionally absolutely stable for decaying solutions;

(b) unconditionally relatively stable for growing solutions.

In addition we may remark that the algorithm is absolutely stable in a growing mode unless $x_i < 1$ and $D_i < 0.5$, a situation only possible for the lowest ionization stage in a rapid ionizing plasma.

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