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THE LIFE HISTORY  
OF IMPURITY ATOMS IN A PLASMA  
POSSESSING A TIME VARYING  
ELECTRON TEMPERATURE AND DENSITY

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THE LIFE HISTORY OF IMPURITY ATOMS IN A PLASMA POSSESSING  
A TIME VARYING ELECTRON TEMPERATURE AND DENSITY

by

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A B S T R A C T

The differential equations describing the life history of an impurity atom in a plasma, through all its stages of ionization, require a numerical solution if the electron density and temperature vary in time in an arbitrary manner. This report outlines some of the physical processes that can be represented by these equations, a method of solution, for which a computer programme has been written, and, in the form of a simple example, the type of problem for which a solution can be obtained. Such calculations are of interest since they enable a cross-check to be effected between measurements of electron temperature and density and observed impurity spectra.

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## 1. INTRODUCTION

1. Virtually all plasmas produced experimentally up to the present time have been contaminated by impurity atoms. In the case of ZETA<sup>(1)</sup>, for example, the main impurity constituents present in a discharge with deuterium as the working gas are carbon, nitrogen and oxygen together with smaller quantities of the liner constituents<sup>(1)</sup>. These are basically an embarrassment to a controlled thermonuclear reactor project in that they constitute an enormous energy sink within the plasma, even in the small quantities in which they generally occur. Energy that should be present as thermal motion of the plasma particles is converted, by collisional excitation, etc., to internal energy of the impurity ions and is then radiated. Since the plasma is in most cases at least partially transparent to this radiation the energy is lost from the system. Again, as an example, in ZETA at moderately high working pressures (~ 5- 10 microns), with a total impurity concentration of about a percent, all the energy discharged into the gas is radiated as fast as it is put in, i.e. at a rate of hundreds of megawatts.

2. This energy loss, however, provides a powerful experimental method for investigating the interior of the plasma since the radiation emitted from a given region of the discharge will be determined by the conditions prevalent there. The process of extrapolation back to the plasma properties from the measurements may, admittedly, be involved and often ambiguous. However, the major advantage of the method is that the introduction of probes and other solid objects into the plasma is not necessary.

3. The radiation emitted by impurities may be divided into two categories - continuum radiation and line radiation. Continuum radiation, emitted over a continuous range of frequencies, is due to electronic transitions between two unbound states (free-free transitions) or from an unbound to a bound state (free-bound transitions). Line radiation on the other hand, emitted only at certain discrete frequencies, is due to bound-bound transitions, i.e. to changes in the internal electron structure of the impurity ions. It is the latter only that will be considered in this report.

4. Measurements of the intensity, as a function of time, of given spectral lines emitted by impurity ions have been made by a great many workers.

Previous attempts<sup>(3-6)</sup> at interpreting the results have been confined to the theoretical analysis of a model in which the assumption of constant electron temperature and density has been made. Independent measurements<sup>(7,8)</sup> of these quantities, however, have been obtained and significant variation can be observed during the discharge period. In the following sections calculations are described in which the restrictions inherent in the above assumption are relaxed, provision being made for any arbitrary variation of density and temperature.

5. The purpose of this report is to outline briefly the physical processes under study (Section 2), and to describe in reasonable detail their mathematical representation and the methods employed in solving the resulting differential equations (Section 3). The equations are solved numerically and a computer programme has been written for this purpose. Details of the input data required and the results obtainable are described in the form of a simple example of the use of the programme (Section 4). Application to a specific experimental situation is not considered. Information of this sort has been<sup>(9)</sup>, and will be, published elsewhere.

6. Details of the programme are not discussed in this report, since they depend to some extent on the computer used. At the present time the programme is written in FORTRAN and could be run with little difficulty on the IBM 704, 7090 and 7030 computers utilizing either the FORTRAN II or S1\* compilers. Access to an automatic graph plotter would also be advantageous, although not essential, the plotting routines at present being written for the BENSON-LEHNER, MODEL J machine. Any person interested in using the programme should contact G.D.Hobbs.

## 2. PHYSICAL PROCESSES

7. The atomic collision processes likely to be predominant in a low pressure gas discharge have been discussed by many authors, for example: McWhirter<sup>(3)</sup> Knorr<sup>(4)</sup> and Post<sup>(5)</sup>. For the calculations described below three only have

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\* S1 is a 'dialect' of FORTRAN written for the IBM 7030 (Stretch) by A.E. Glennie et al of A.W.R.E., Aldermaston, in conjunction with IBM (United Kingdom).

been included, these being generally accepted as the most important.

- (1) Collisional ionization of an atom or ion by an electron.
- (2) Recombination of an ion with an electron.
- (3) Collisional excitation of an atom or ion by an electron.

8. In calculating the rates at which these processes proceed in a small volume of the plasma it has been assumed that the electron component of the gas has, locally, a Maxwellian distribution of velocities characterized by a temperature  $T$ . Thus, if  $f(v)dv$  is the fraction of electrons with velocities in the range  $v$  to  $v + dv$ ,

$$f(v) = 4\pi \left( \frac{m}{2\pi kT} \right)^{\frac{3}{2}} v^2 e^{-\frac{mv^2}{2kT}},$$

where  $m$  is the electron mass and  $k$  is Boltzmann's constant.

9. In addition to the collision processes, provision has been made for loss and injection of ions in order to take into account any lack of containment of the plasma.

10. The model, then, allows for an atom (or ion) to be injected into the plasma, (or in the case of the neutral atom, to be there from the start), where it will undergo ionization, resulting in the loss of one or more electrons; recombination, resulting in the gain of one or more electrons; excitation, resulting in the emission of line radiation; and finally perhaps ejection from the volume to lose its identity on the walls of the containing vessel. The relative rates with which these different processes proceed depend on their individual cross-sections and probabilities and the way in which these vary with  $T$  and the electron density  $n_e$ .

11. In principle the model applies only to an infinitesimal volume of space. To apply it to a finite discharge volume would lead, if done rigorously, to complex integrals. However, since experimental determinations of  $n_e$  and  $T$  as functions of space and time are not easy to come by, it is not unreasonable to assume them spatially uniform, together with all other plasma properties, and apply the model to the discharge as a whole.

12. It may be mentioned here that each process is treated by a self-contained sub-programme. This makes the programme flexible since one or more of the existing sub-programmes may, if desired, be replaced by others which



take into account different physical situations (e.g. substitution of a mono-energetic electron stream in place of the present Maxwellian velocity distribution), leaving the major part of the programme unaffected.

13. In all that follows the term 'ion' should, in general, be interpreted as 'atom or ion'.

### IONIZATION

14. The physics of ionization by electron impact is complex<sup>(10)</sup>. The simplest process conceivable is that of an electron impinging on an ion with sufficient energy to eject an outer bound electron from the ground state directly into the continuum. The energy required to do so must be at least  $E_0$ , the first ionization potential of the ion. More complicated processes are easily envisaged; for example, excitation of the ion to an intermediate bound state by one electron followed by ionization out of that state by a second electron. Clearly the individual energies required by these two electrons need not be as high as in the case of the simple process. To include all such processes would be an enormous task and the form in which ionization has been treated in this report is therefore somewhat generalized, the detailed structure being left at the disposal of the individual user.

15. Three properties are assigned to the ionization cross-section for an individual collision, when expressed as a function of energy. It must vanish below an ionization potential  $E_0$ , have at least one maximum and fall off asymptotically as  $1/E$ . These properties have been embodied in a single analytic form.

$$\begin{aligned} \sigma(E) &= 0, & E &\leq E_0; \\ &= A \frac{E - E_0}{E^2} + B \frac{(E - E_0)^2}{(E + E_1)^3}, & E &\geq E_0. \end{aligned} \quad \dots (1)$$

The parameters  $A$ ,  $B$ ,  $E_0$  and  $E_1$  can be chosen to fit the data relevant to the particular ion under consideration. In particular, if  $B = 0$  and  $A = \alpha/E_0$ , where  $\alpha$  is a given numerical constant, the 'classical' cross-section<sup>(11)</sup> for ionization is obtainable.

16. The total rate of ionization of a particular ion, denoted by a subscript  $i$ , is given by:-

$$\frac{dn_i}{dt} = -n_e n_i S_i \quad \dots (2)$$



where  $S_i = \langle \sigma_i v \rangle$  is the ionization coefficient and the brackets denote averaging over the Maxwellian velocity distribution, i.e.

$$S_i = \langle \sigma_i v \rangle = \int_{v_{oi}}^{\infty} \sigma_i v f(v) dv, \quad \dots (3)$$

the lower limit being taken as  $v_{oi} = (2E_{oi}/m)^{\frac{1}{2}}$ , below which  $\sigma_i$  vanishes. The coefficient can be written in terms of exponential integrals<sup>(12)</sup> and its calculation is discussed in more detail in Appendices 1 and 2.

### RECOMBINATION

17. Since recombination is physically just the converse of ionization it would not be expected to be any less complex. Two basic processes have been assumed to contribute to the total recombination coefficient  $\alpha$ , in terms of which the total rate of recombination is given by:

$$\frac{dn_i}{dt} = -n_e n_i \alpha_i.$$

18. The first, radiative recombination, is defined by the equation

$$A_Z + e \rightarrow A_{Z-1} + h\nu,$$

where  $A_Z$  denotes an ion carrying a net charge  $+Ze$ . The theory of radiative recombination for hydrogen-like ions has been successfully analysed but a complete mathematical description of the process for anything more complex has yet to be obtained. In view of this it has been assumed that the recombination coefficient for an ion of charge  $Z$  may, as a reasonable approximation, be replaced by that for the hydrogen-like ion of identical charge. This coefficient, when averaged over a Maxwellian velocity distribution at a temperature  $T$  can be written<sup>(13)</sup> in the form:-

$$\alpha_R(Z, T) = 9.56 \times 10^{-14} \frac{Z^2}{T^{\frac{1}{2}}} \left\{ G(n_1, Z, T) + \sum_{n=1}^{n_1-1} \frac{2}{n} F(x_n) \right\}, \quad \dots (4)$$

where

$$G(n_1, Z, T) = \frac{F(x_{n_1 - \frac{1}{2}})}{x_{n_1 - \frac{1}{2}}} + \ln(x_{n_1 - \frac{1}{2}}) + \ln \gamma,$$

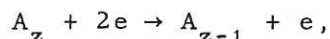
$$F(x) = -x e^x \hat{E}i(-x),$$

$$x_n = 13.60 \frac{Z^2}{n^2 T}$$

and, if  $T$  is in eV,  $\alpha_R$  is in  $\text{cm}^3/\text{sec}$ . The constant  $\ln \gamma = 0.577216$  and  $\hat{E}i(-x)$  is the exponential integral<sup>(12)</sup> (see also Appendix 2). The series represents a summation over the lowest  $n_1 - 1$  energy levels of the ion and  $G(n_1, Z, T)$  is

an integral representation of the summation over the remaining levels. The recommended value of 4 has been adopted for  $n_1$  in these calculations.

19. The second process, three body recombination, is defined by the equation



the second electron carrying off the excess energy. Until recently this process had been thought to be negligible at the temperatures and densities encountered in low pressure gas discharges. However a new study<sup>(14)</sup> of the subject has shown this conjecture to be untrue under certain circumstances. Its effect on the total recombination coefficient  $\alpha$  has been included, rather crudely, as a factor  $H$  multiplying  $\alpha_R$ , i.e.

$$\alpha = H\alpha_R \quad \dots (5)$$

This factor, determined only by the average density and temperature, has been assumed constant throughout a calculation. In those cases in which there is an appreciable order of magnitude variation of  $n_e$  and  $T$  during the discharge period this approximation may be invalid.

#### EXCITATION

20. The phenomenon observed experimentally is the variation of intensity of a spectral line emitted by a specific ion. The process assumed to give rise to such a line is collisional excitation of the ion from an initial to a higher state followed immediately, that is on a time scale short compared to any other physical process under consideration, by a spontaneous radiative decay. The population density of the initial state, which will in general be the ground state, is assumed to exactly equal the ion number density  $n_i$ . If the energy separation of the initial and excited levels is  $\chi$ , then the rate of excitation, equal in this approximation to the rate of emission (radiated intensity), will be proportional to the excitation coefficient, which on averaging over the Maxwellian velocity distribution, can be written<sup>(14)</sup>

$$X = \text{Const} \times (kT)^{-\frac{1}{2}} \exp(-\chi/kT). \quad \dots (6)$$

This expression is based on a cross-section for collisional excitation given by Seaton<sup>(15)</sup>. The value of the constant is irrelevant unless absolute intensities are required. The programme discussed in this report was designed to give the variation of radiated intensity with time, not its



absolute magnitude. Hence, the constant has been chosen to provide a convenient normalization for the tabulation and plotting of the results. It should be noted that  $\chi$  is not the energy  $h\nu$  of the radiated photons unless the transition involved is back to the initial state.

21. Finally, the total radiated intensity emitted in a specific line will be given by:

$$I_i = n_e n_i X_i , \quad \dots (7)$$

the subscript  $i$  again denoting the particular ion. The radiation will be emitted in all directions and before comparison with the corresponding experimental data some geometrical correction factor may need to be taken into consideration. A typical example of such a correction is provided when the volume observed does not remain a constant fraction of the whole, as in a pinch discharge viewed by a constant aperture instrument.

#### LOSS AND INJECTION

22. Impurities appearing in a gas discharge plasma arise from two main sources, those already present in the working gas and those coming from the walls of the containment vessel. The latter may be injected into the plasma during the entire period over which the discharge lasts. In practice the rate of injection  $\Lambda$  varies with time but for simplicity it has been included in these calculations as a constant, a different rate being available for each type of ion.

23. Frequently not only do impurities stream in from the walls but, due to instability, etc., plasma is lost to the walls of the containing vessel<sup>(5)</sup>. It would be unreasonable to expect the working gas to leave the system without the attendant impurities. Thus provision has been made to represent, again in a simple manner, the loss of impurity ions. The rate of loss has been assumed to be proportional to the number present, the constant of proportionality  $\lambda$  being independent of time but, if necessary, different for each type of ion.

24. Finally, the total rate of change of ions due to the combined loss and injection processes can be written in the form:-

$$\frac{dn_i}{dt} = \Lambda_i - \lambda_i n_i \quad \dots (8)$$

### 3. THE BASIC EQUATIONS AND THEIR SOLUTION

#### DEFINITION

25. The basic equations governing the life history of an impurity atom through all its stages of ionization have been written down and discussed in previous papers<sup>(3,5,6)</sup>. They are

$$\left. \begin{aligned} \frac{dn_1}{dt} &= -n_e n_1 S_1 + n_e n_2 \alpha_2 + \Lambda_1 - \lambda_1 n_1, \\ \frac{dn_i}{dt} &= n_e n_{i-1} S_{i-1} - n_e n_i S_i - n_e n_i \alpha_i + n_e n_{i+1} \alpha_{i+1} + \Lambda_i - \lambda_i n_i, \\ \frac{dn_k}{dt} &= n_e n_{k-1} S_{k-1} - n_e n_k \alpha_k + \Lambda_k - \lambda_k n_k, \end{aligned} \right\} \dots (9)$$

where  $i = 2, 3, \dots, k-1$ ,  $n_1$  is the number density of neutral atoms,  $n_2$  that of singly ionized atoms,  $n_3$  that of doubly ionized atoms, etc., and  $n_k$  is the number density of 'fully stripped ions'. The 'fully stripped ion' is defined for the purposes of these calculations as being that ion for which the maximum ionization rate likely to be encountered during the calculation is negligible compared to the recombination rate of the  $k+1$ th ion, and for which  $S_k$  can be set equal to zero in order to terminate the set of equations. The significance of the various terms in equations (9) can readily be inferred by reference to the previous section.

26. Adding the  $k$  equations (9) together and defining  $n_0(t) = \sum_{i=1}^k n_i(t)$  yields

$$\frac{dn_0}{dt} = \frac{d}{dt} \sum_{i=1}^k n_i(t) = \sum_{i=1}^k \Lambda_i - \sum_{i=1}^k \lambda_i n_i, \quad \dots (10)$$

which, on integration from 0 to  $t$  gives

$$n_0(t) = n_0(0) + \left( \sum_{i=1}^k \Lambda_i \right) t - \sum_{i=1}^k \lambda_i \int_0^t n_i(t') dt'. \quad \dots (11)$$

This just states that the total number of ions present at any time  $t$  is equal to the sum of those present initially,  $n_0(0)$ , and those injected during the interval 0 to  $t$ , less those lost from the system in the same period. As would be expected the atomic collision processes do not contribute to changes in the total number of ions and if  $\Lambda_i = \lambda_i = 0$ , for all  $i$ , this number is conserved.

27. If all the  $\lambda_i$  are equal, i.e.  $\lambda_i = \lambda$ , equation (10) may be solved analytically, the solution being

$$n_0(t) = \frac{\Lambda}{\lambda} + \frac{\lambda n_0(0) - \Lambda}{\lambda} e^{-\lambda t},$$



where  $\Lambda = \sum_{i=1}^k \Lambda_i$ , and is the total rate of particle injection. The solution possesses the following properties:

- (a)  $\lim_{t \rightarrow \infty} n_0(t) = \Lambda/\lambda$ .
- (b) If  $\Lambda > \lambda n_0(0)$ ,  $n_0(t)$  increases monotonically to the limit (a).
- (c) If  $\Lambda < \lambda n_0(0)$ ,  $n_0(t)$  decreases monotonically to the limit (a).
- (d) If  $\Lambda = \lambda n_0(0)$ ,  $n_0(t)$  remains constant at  $n_0(0)$ .

28. The boundary conditions appropriate to the set of equations (9) are determined by the assumption that initially all the impurity atoms are in an unionized state. Thus, given the initial concentration  $n_0(0)$ , the boundary conditions become

$$\left. \begin{aligned} n_i &= n_0(0), \\ n_i &= 0, \quad i \neq 1. \end{aligned} \right\} \text{ at } t = 0$$

These may not be valid if an intense preheating mechanism is used which results in a significant degree of ionization in the gas.

#### SOLUTION

29. Solutions of these equations have been obtained under two extreme sets of conditions. The first and simplest entails neglecting loss and injection and insisting that the electron temperature  $T$ , and hence the coefficient  $S_i$  and  $\alpha_i$ , be independent of time. Solutions of this type can be obtained by analytic methods and have been discussed in earlier works<sup>(3-5)</sup>. For completeness, and for those who may be interested in studying them, a simple method of solution which is particularly suitable for automatic digital computers is set out in Appendix 3.

30. The other class of solutions considered takes into account not only the loss and injection processes but also the possibility of  $n_e$  and  $T$  varying with time in an arbitrary manner. Under these circumstances analytic integration of the equations becomes impossible and resort must be made to numerical techniques. The method of integration adopted was that of Runge-Kutta<sup>(15)</sup>. This was chosen in spite of its inherent instability characteristics firstly, because a well tried fourth order sub-programme was already in existence and secondly because a simple rearrangement of the differential equations enabled the instability difficulties to be overcome.

31. The Runge-Kutta procedure is developed from a Taylor series expansion of

the solutions of the differential equations. It is an unfortunate fact that equations (9) under certain circumstances, possess solutions that to a first approximation (e.g. see Appendix 3) can be expressed as a sum of exponentials with widely differing negative exponents. It is known that the Runge-Kutta method is susceptible to instability on encountering such solutions unless a very small step length is used. The magnitude of this step length is determined by the ability of the method to make a valid Taylor series expansion of the exponential with the largest exponent, i.e. in general it is determined by the term contributing least to the total solution.

32. To overcome these difficulties the integration is done in two successive stages. In the first stage equations (9) are integrated from  $t = 0$  until  $n_1$  has fallen to a small fraction of its initial value (all the other  $n_i$  have normally attained non-zero values by then). It is from this latter point onwards that instability is likely to occur and at which the second stage of the integration commences. Dividing equations (9) throughout by  $n_1, n_i$  and  $n_k$  respectively, and defining  $y_i$  by

$$y_i = \ln n_i, \text{ all } i,$$

the set of differential equations may be rewritten in the form

$$\left. \begin{aligned} \frac{dy_1}{dt} &= - (n_e S_1 + \lambda_1) + n_e a_2 \exp(y_2 - y_1) + \Lambda_1 \exp(-y_1), \\ \frac{dy_i}{dt} &= n_e S_{i-1} \exp(y_{i-1} - y_i) - [n_e (S_i + a_i) + \lambda_i] + n_e a_{i+1} \exp(y_{i+1} - y_i) + \Lambda_i \exp(-y_i), \\ \frac{dy_k}{dt} &= n_e S_{k-1} \exp(y_{k-1} - y_k) - (n_e a_k + \lambda_k) + \Lambda_k \exp(-y_k). \end{aligned} \right\} (12)$$

33. These equations have solutions that are essentially algebraic and can be handled without any difficulty by the Runge-Kutta technique. Thus in the second stage it is these equations, not equations (9) that are integrated.

34. Even though much computer time has to be expended in evaluating the many exponential factors it was not difficult to obtain a ten-fold time saving over the direct integration of equations (9) using such a step length as to ensure stability. (Simple methods, such as linear extrapolation,  $n_i(t + \delta t) = n_i(t) + \delta t \, dn_i/dt$ , proved to be equally slow.) The two stage scheme is necessary because all except the first of the  $y_i$  became singular at  $t = 0$  by virtue of the boundary conditions.



## STEP LENGTH AND ACCURACY

35. Since an approximate analytic solution can be found for equations (9) during the first stage of the integration, the initial step length  $\delta t$  can be calculated quite simply. Near  $t = 0$ ,  $n_i \ll n_1$  for  $i \geq 2$ , and the only equation of importance reduces to

$$\frac{dn_1}{dt} = -[n_e S_1 + \lambda_1] n_1 + \Lambda_1.$$

Provided  $n_e$  and  $S_1$  (i.e.  $T$ ) do not vary too rapidly over the first few steps, the solution of this equation can be written

$$n_1(t) = n_0(0)e^{-t/\tau_0} + \Lambda_1 \tau_0(1 - e^{-t/\tau_0}) \\ \approx n_0(0)(1 + t/\tau_1)$$

where  $\tau_0 = (n_e S_1 + \lambda_1)^{-1}$  and  $\tau_1 = \tau_0(1 - \Lambda_1 \tau_0/n_0(0))^{-1}$ . Thus if  $\delta t$  is chosen such that  $\delta t \ll \tau_1$  the integration will be sufficiently accurate. In practice a constant step length of  $\tau_1/100$  ensures a tolerably small error during the integration of equations (9).

36. In the second stage, i.e. during the integration of equations (12), the step length is recalculated at every step in such a way as to obtain the fastest integration commensurate with a high degree of accuracy. In all,  $k+1$  equations are integrated simultaneously to give  $n_0(t)$  and  $n_i(t)$ ,  $i = 1, 2, \dots, k$  and the accuracy of each step is investigated by making a comparison between  $n_0(t)$  computed from equation (10) and  $n_0(t)$  computed from  $\sum_{i=1}^k n_i$ .

The procedure for making this comparison is as follows:-

- (1) At the end of the  $m-1$ th successful step the solutions  $n_0^{(m-1)}$  and  $n_i^{(m-1)}$ ,  $i = 1, 2, \dots, k$  are known and the parameters  $\Sigma^{(m-1)}$  and  $\delta_1^{(m-1)}$  have been computed, where

$$\Sigma^{(m-1)} = \sum_{i=1}^k n_i^{(m-1)}$$

and

$$\delta_1^{m-1} = |n_0^{(m-1)} - \Sigma^{(m-1)}|,$$

the actual error present in the solution at this point.

- (2) The step length for the  $m$ th step is computed from  $\delta t^{(m)} = \delta t^{(m-1)}$  or, at every fifth successful step, from  $\delta t^{(m)} = 2\delta t^{(m-1)}$ .

- (3) The  $k+1$  equations are integrated by the Runge-Kutta sub-programme.

- (4) The parameters  $\delta_1^{(m)}$  and  $\delta_2^{(m)}$  are calculated, where

$$\delta_2^{(m)} = |\delta_1^{(m)} - \delta_1^{(m-1)}|,$$

the change in the error incurred during the  $m$ th step.

- (5) If  $\delta_2^{(m)} \leq \epsilon$ , a prescribed error, the integration is considered

successful and the next step is attempted.

(6) If  $\delta_2^{(m)} > \varepsilon$ , the step length is halved and the integration repeated from (3). (The calculation is automatically terminated if this occurs more than 10 times in attempting one step.)

37. In this way the rate of increase of the discrepancy between  $n_0(t)$  and  $\sum_{i=1}^k n_i(t)$  is maintained small. The permitted error  $\varepsilon$  is chosen so that the maximum total error  $N\varepsilon$ , where  $N$  is the total number of successful time steps, at the end of the calculation, i.e. the number of particles gained or lost due to arithmetical inaccuracies, is very much less than  $n_0(0)$ . In the existing version of the programme  $n_0(0) = 10^4$  and  $\varepsilon = 10^{-3}$ , hence an accuracy of 0.01% is maintained if  $N = 10^3$  and, since the maximum number of steps permitted is  $2 \times 10^4$ , the overall maximum error is 0.2%.

38. Attempts to monitor  $\delta_1^{(m)}$  itself and to apply a constraint of the form  $\delta_1^{(m)} < \varepsilon_1$ , some other prescribed error, proved completely unsuccessful. It was found that, during the first few steps, the step length adjusted itself to the maximum value possible, resulting in a rapid build-up of  $\delta_1^{(m)}$  to within a small fraction of its maximum value  $\varepsilon_1$ . From that point onwards  $\delta t$  was forced to become very small in order to ensure that  $\delta_1^{(m)}$  did not exceed that value, the net effect being to slow the calculation down considerably.

39. The criterion discussed above, while being successful during the integration of equations (12), cannot be applied to equations (9). These equations possess the property that, if the physical loss and injection processes are omitted, the total number of ions is conserved irrespective of the stability or accuracy of the solution.

#### 4. AN EXAMPLE

40. This section summarises the data required in order to use the programme and the results obtainable. The summary has been drawn up in the form of a simple example, the details of which have been chosen to illustrate the facilities available to the user.

41. The discharge considered possessed the measured temperature and density variation illustrated in Fig.1. The total period over which measurements could be made was 5 milliseconds (msecs). The data of this figure was



supplied to the programme in the form of two tables, one, with 79 entries, of temperature against time, and the other, with 73 entries, of density against time. It was not necessary for the intervals of tabulation to be identical in the two tables.

42. The impurity investigated was nitrogen which was assumed present initially at a density of  $10^{11}$  atoms/cc. In addition neutral nitrogen was assumed to be injected into the discharge from the walls at a rate of  $2 \times 10^{10}$  atoms/cc/msec. Since the programme always sets the initial neutral density to  $10^4$ /cc, the injection rate must be scaled to bring it into proportion. Thus the value of  $\Lambda_1$  used for the input data was corrected to  $2 \times 10^6$  atoms/cc/sec ( $2 \times 10^3$ /cc/msec). An experimentally measured ion containment time of 1 msec was adopted, giving a fractional loss rate coefficient  $\lambda$ , the same for all ions, of  $10^3$ /sec.

43. The details of the ionization cross-sections were based on data taken from Allen<sup>(11)</sup>. The shape of  $\sigma(E)$  is shown in Fig.2, the maximum,  $\sigma_{\max}$ , being given by

$$\sigma_{\max} = bn \pi a_0^2 (E_0/E_{OH})^{-2} \text{ cm}^2,$$

where

$$\pi a_0^2 = 8.80 \times 10^{-17} \text{ cm}^2,$$

$$bn = 0.8 \text{ for one outer electron,}$$

$$= 2.0 \text{ for more than one outer electron,}$$

and

$$E_{OH} = 13.56 \text{ eV, is the first ionization potential}$$

of atomic hydrogen. From this form of the cross-section the set of ionization parameters listed in Table I was derived.

TABLE I

i	Z	$A_i$ ( $\text{cms}^2\text{eV}$ )	$B_i$ ( $\text{cms}^2\text{eV}$ )	$E_{0i}$ (eV)	$E_{1i}$ (eV)
1	0	$2.6403 \times 10^{-15}$	$2.1997 \times 10^{-14}$	14.540	12.276
2	1	$1.2967 \times 10^{-15}$	$1.0804 \times 10^{-14}$	29.605	24.994
3	2	$8.0947 \times 10^{-16}$	$6.7440 \times 10^{-15}$	47.426	40.040
4	3	$4.9567 \times 10^{-16}$	$4.1297 \times 10^{-15}$	77.450	65.388
5	4	0	0	-	-

The termination of the table at  $i = 5$  was justified by investigating the relative magnitude of the ionization and recombination coefficients to be expected in the calculations.

44. A value of 4.5 was adopted for the factor H in order to represent the excess recombination due to three body processes. The excitation potentials for the particular spectral line of each ion to be studied were  $\chi_1 = 10.00$  eV,  $\chi_2 = 11.39$  eV,  $\chi_3 = 12.47$  eV,  $\chi_4 = 51.85$  eV and  $\chi_5 = 9.97$  eV.

45. The output from the programme is in two forms - numerical and graphical. The former, in addition to a listing of the input data, consists of two tables; a tabulation of T,  $n_e$ ,  $n_0$ ,  $n_1$ ,  $n_2$ , ...  $n_k$  against time, and a list of normalized spectral line intensities at the same time intervals. The latter consists of two graphs displaying the contents of each of the two tables.

46. The graphical results obtained for this particular example are exhibited in Figs.3 and 4. Interesting points to note are;

(1) The rapid decay of the neutral number density followed by the peaks  $P_{II}$  and  $P_{III}$  demonstrating the passage of the nitrogen atoms through their successive stages of ionization, leading after about 1 msec to a small proportion of N IV and a very small proportion of NV (not shown).

(2) The peaks  $P'_{II}$ ,  $P'_{III}$  and  $P'_{IV}$  due to recombination as the electron temperature falls during the latter half of the calculation, leading back ultimately to neutral nitrogen. In fact NI begins to reappear during the last millisecond.

(3) The steady exponential fall in the total number of particles to its equilibrium value  $\Lambda/\lambda$  at which loss and injection just balance.

(4) The considerable difference in shape between the number densities and their corresponding line intensities. In particular the effect of the falling excitation coefficients (i.e. falling T) in masking nearly all the features displayed by the number densities during the latter half of the calculation.

47. The above example illustrates all the details of the input and output data except the restrictions that have to be imposed on certain quantities.

These are listed below:-

(1) The total number of ions k may not exceed 12.

(2) The number of entries in each of the two tables T and  $n_e$  against time may not exceed 100.

(3) The maximum number of entries in the final tables of  $n_i$  against time will not exceed 1000. If this number is reached the calculation is terminated automatically.

## 5. ACKNOWLEDGEMENTS

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APPENDIX 1  
THE CALCULATION OF IONIZATION COEFFICIENTS

48. The ionization coefficient is defined by

$$S = \int_{v_0}^{\infty} \sigma v f(v) dv, \quad (\text{A.1.1})$$

where

$$\sigma = A \frac{E - E_0}{E^2} + B \frac{(E - E_0)^2}{(E + E_1)^3}, \quad E \geq E_0, \quad (\text{A.1.2})$$

$$f(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} v^2 e^{-\frac{mv^2}{2kT}}, \quad (\text{A.1.3})$$

$$v = (2E/m)^{\frac{1}{2}}, \quad \text{and in particular } v_0 = (2E_0/m)^{\frac{1}{2}}.$$

After a certain amount of labour  $S$  can be reduced to the form

$$S = \left(\frac{8}{\pi m k T}\right)^{\frac{1}{2}} \{A[x_0 \mathcal{E}_i(-x_0) + e^{-x_0}] + B[R_1 e^{-x_0} + R_2 e^{x_1} \mathcal{E}_i(-x_0 + x_1)]\}, \quad (\text{A.1.4})$$

where

$$R_1 = 1 + x_0 + \frac{5}{2} x_1 + \frac{1}{2} x_1 (x_0 + x_1),$$

$$R_2 = 2x_0 + 3x_1 + (x_0 + 3x_1)(x_0 + x_1) + \frac{1}{2} x_1 (x_0 + x_1)^2,$$

$$x_0 = E_0/kT, \quad x_1 = E_1/kT$$

and

$$\mathcal{E}_i(-x) \equiv \int_x^{\infty} \frac{e^{-z}}{z} dz. \quad (\text{A.1.5})$$

49. In the limit of small  $T$ , i.e. large  $x_0$  and  $x_1$ , difficulty has been experienced due to the cancellation of terms such as  $x_0 \mathcal{E}_i(-x_0)$  and  $e^{-x_0}$  to a large number of figures resulting in sizable errors in computing  $S$ . In order to overcome this, asymptotic expansions have been introduced in the following manner. Successive integration by parts yields

$$\mathcal{E}_i(-x) \sim \frac{e^{-x}}{x} \left[1 - \frac{1!}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} + \dots\right].$$

Thus

$$\begin{aligned} x_0 \mathcal{E}_i(-x_0) + e^{-x_0} &= e^{-x_0} [x_0 e^{x_0} \mathcal{E}_i(-x_0) + 1] \\ &\sim \frac{e^{-x_0}}{x_0} \left[1 - \frac{2!}{x_0} + \frac{3!}{x_0^2} - \dots\right]. \end{aligned}$$

Similarly, if  $x_2 = x_0 + x_1$ ,

$$\begin{aligned} R_1 e^{-x_0} + R_2 e^{x_1} \mathcal{E}_i(-x_2) &= e^{-x_0} [R_1 + R_2 e^{x_2} \mathcal{E}_i(-x_2)] \\ &\sim e^{-x_0} \left\{ \left[R_1 - \frac{R_2}{x_2}\right] + \frac{R_2}{x_2^2} \left[1 - \frac{2!}{x_2} + \frac{3!}{x_2^2} - \dots\right] \right\}. \end{aligned}$$

Thus, since  $R_1 - R_2/x_2 = -[1 + \frac{1}{2}x_1 + \frac{x_1}{x_2}]$ , and defining the series,

$$P(x) = \frac{1!}{x} - \frac{2!}{x^2} + \frac{3!}{x^3} - \dots = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} n!}{x^n},$$

the asymptotic form of  $S$  can be written

$$S \sim \left(\frac{8}{\pi m k T}\right)^{\frac{1}{2}} \{A P(x_0) + B \frac{R_2}{x_2} P(x_2) - B(1 + \frac{x_1}{2} + \frac{x_1}{x_2})\} e^{-x_0}. \quad (\text{A.1.6})$$

## APPENDIX 2

### THE CALCULATION OF EXPONENTIAL INTEGRALS

50. The Exponential Integral is defined<sup>(12)</sup> by

$$- \mathcal{E}i(-x) = \int_x^\infty \frac{e^{-z}}{z} dz, \quad 0 < x < \infty.$$

It can be represented by the absolutely convergent series

$$\begin{aligned} \mathcal{E}i(-x) &= \ln \gamma x - x + \frac{x^2}{2!2} - \frac{x^3}{3!3} + \dots \\ &= \ln \gamma x + \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n!n}, \end{aligned}$$

where  $\ln \gamma = 0.577215665$ , the Euler-Mascheroni constant.

51. Although convergent for all positive  $x$ , there is a serious cancellation of significant figures for large values of  $x$ . Thus the series has only been used to compute  $\mathcal{E}i(-x)$  for  $x \leq 1$ , sufficient terms being taken to ensure a percentage accuracy of  $10^{-5}$ .

52. For  $x > 1$ , an approximation<sup>(17)</sup> in which  $xe^x \mathcal{E}i(-x)$  is expressed as the ratio of two quartics has been used. i.e.

$$- xe^x \mathcal{E}i(-x) = \frac{x^4 + a_3 x^3 + a_2 x^2 + a_1 x + a_0}{x^4 + b_3 x^3 + b_2 x^2 + b_1 x + b_0}$$

where

$$\begin{aligned} a_0 &= 0.2677737343, & b_0 &= 3.9584969228; \\ a_1 &= 8.6347608925, & b_1 &= 21.0996530827; \\ a_2 &= 18.0590169730, & b_2 &= 25.6329561486; \\ a_3 &= 8.5733287401, & b_3 &= 9.5733223454. \end{aligned}$$

This function represents the Exponential integral to a percentage accuracy of  $2 \times 10^{-6}$  in the range  $1 \leq x < \infty$ .



### APPENDIX 3

#### A SIMPLE ANALYTIC SOLUTION

##### FORMAL SOLUTION

53. If loss and injection processes are neglected, i.e.  $\lambda_i = \Lambda_i = 0$ , equations (9) can be rewritten in the form

$$\left. \begin{aligned} \frac{dn_1}{d\tau} &= -n_1 S_1 + n_2 a_2 \\ \frac{dn_i}{d\tau} &= n_{i-1} S_{i-1} - n_i (S_i + a_i) + n_{i+1} a_{i+1} \\ \frac{dn_k}{d\tau} &= n_{k-1} S_{k-1} - n_k a_k, \end{aligned} \right\} \quad (\text{A.3.1})$$

where the new variable  $\tau$  is given by

$$\tau = \int_0^t n_e(t') dt'.$$

54. It is now formally advantageous to take the Laplace Transform of equations (A.3.1) and express the result in matrix form:

$$\mathcal{D}_k(p) \tilde{N}_k(p) = \tilde{n}_0, \quad (\text{A.3.2})$$

where

$$\mathcal{D}_k(p) = \begin{bmatrix} p+A_1 & -C_2 & 0 & 0 \\ -B_1 & p+A_2 & -C_3 & 0 \\ 0 & -B_2 & p+A_3 & 0 \\ 0 & 0 & 0 & p+A_k \end{bmatrix},$$

$$\tilde{N}_k(p) = \begin{bmatrix} \tilde{n}_1(p) \\ \tilde{n}_2(p) \\ \vdots \\ \tilde{n}_k(p) \end{bmatrix}, \quad \tilde{n}_0 = \begin{bmatrix} n_0(o) \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

and

$$\begin{aligned} A_1 &= S_1; \quad A_k = a_k; \quad A_i = S_i + a_i, \quad 2 \leq i \leq k-1; \\ B_i &= S_i, \quad 1 \leq i \leq k-1; \\ C_i &= a_i, \quad 2 \leq i \leq k. \end{aligned}$$

The Laplace Transform of  $n_i(\tau)$  is defined by

$$\tilde{n}_i(p) = \int_0^\infty n_i(\tau) e^{-p\tau} d\tau$$

and  $n_0(o)$  is the initial value of  $n_1(\tau)$ .

55. Equation (A.3.2) can be solved with the aid of Cramer's rule, the solution having the form

$$\tilde{n}_j(p) = \frac{E_{jk}(p)}{D_k(p)},$$

where  $D_k(p)$  is the determinant of  $\mathcal{D}_k(p)$  and  $E_{jk}$  is formed from  $D_k(p)$  by replacing its  $j$ th column by the column vector  $\tilde{n}_0$ , i.e.

$$E_{jk}(p) = \begin{vmatrix} p+A_1 & -C_2 & 0 & & 0 & n_0(o) & 0 & 0 \\ -B_1 & p+A_2 & -C_3 & & & & & 0 \\ 0 & -B_2 & p+A_3 & & & & & 0 \\ & & & & & & & \\ 0 & & & p+A_{j-1} & 0 & 0 & & 0 \\ 0 & & & -B_{j-1} & 0 & -C_{j+1} & & 0 \\ 0 & & & 0 & 0 & p+A_{j+1} & & 0 \\ & & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & p+A_k \end{vmatrix}.$$

Inverting the Laplace Transform,

$$n_j(\tau) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{E_{jk}(p)}{D_k(p)} e^{p\tau} dp,$$

the contour  $\gamma$  being chosen to lie to the right of all the poles of the integrand. These are situated at the zeros of the determinant  $D_k(p)$  and are defined by

$$D_k(-p_i) = 0.$$

In terms of the  $p_i$

$$D_k(p) = \prod_{\ell=1}^k (p + p_\ell).$$

The residue from the  $i$ th pole is given by

$$R_i = \frac{E_{jk}(-p_i)}{\prod_{\ell \neq i} (p + p_\ell)}.$$

Thus

$$n_j(\tau) = \sum_{i=1}^k \frac{E_{jk}(-p_i)}{\prod_{\ell \neq i} (p + p_\ell)} e^{-p_i \tau}. \quad (A.3.3)$$

This is the formal solution of equation (A.3.1). It has been obtained in this way due to the relative ease in which, once the roots  $p_i$  have been found, the coefficients of the series may be evaluated.

# THE ROOTS OF $D_k(p) = 0$

56. Standard numerical procedures are available for the extraction of the zeros of a given function. Frequently it is advantageous to express the function in the form of a polynomial. For the case of this particular determinant the transformation is straight forward. Thus, if

$$D_k(p) = \sum_{m=0}^k g_{km} p^m,$$

the coefficients  $g_{km}$  are given by

$$g_{km} = \frac{1}{m!} D_k^{(m)}(0),$$

where  $D_k^{(m)}(p)$  is the  $m$ th derivative of  $D_k(p)$ .

57. Due to the tri-diagonal nature of  $D_k$  it can be evaluated rapidly with the aid of certain recurrence relations. Consider the  $n \times n$  determinant  $D_n(p)$  where  $n$  lies in the range  $0 \leq n \leq k$  and  $D_n(p)$  is defined by

$$D_n(p) = \begin{vmatrix} p+A_1 & -C_2 & 0 & & 0 \\ -B_1 & p+A_2 & -C_3 & & 0 \\ 0 & -B_2 & p+A_3 & & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & & p+A_n \end{vmatrix}.$$

$$\begin{aligned} \text{Then } D_0 &= 1, \\ D_1 &= p+A_1 \end{aligned}$$

$$\text{and } D_n(p) = (p+A_n)D_{n-1}(p) - B_{n-1}C_n D_{n-2}(p), \quad n \geq 2.$$

Differentiation with respect to  $p$  gives

$$D_0^{(0)} = 1; \quad D_0^{(m)} = 0, \quad m \geq 1$$

$$D_1^{(0)} = p+A_1; \quad D_1^{(1)} = 1; \quad D_1^{(m)} = 0, \quad m \geq 2$$

$$\text{and } D_n^{(m)}(p) = (p+A_n)D_{n-1}^{(m)}(p) - B_{n-1}C_n D_{n-2}^{(m)}(p) + mD_{n-1}^{(m-1)}(p), \quad n \geq 2, \quad m \geq 0.$$

Thus, in the limit  $p = 0$ , the coefficient  $g_{km}$  may be generated from the recurrence relation

$$D_0^{(0)} = 1; \quad D_0^{(m)} = 0, \quad m \geq 1$$

$$D_1^{(0)} = A_1; \quad D_1^{(1)} = 1; \quad D_1^{(m)} = 0, \quad m \geq 2;$$

$$\text{and } D_n^{(m)}(0) = A_n D_{n-1}^{(m)}(0) - B_{n-1} C_n D_{n-2}^{(m)}(0) + m D_{n-1}^{(m-1)}(0), \quad 2 \leq n \leq k, \quad 0 \leq m \leq n.$$



## EVALUATION OF $E_{jk}(p)$

58. Having extracted the roots of  $D_k(p) = 0$ , the only significant problem remaining is the calculation of  $E_{jk}(p)$  at  $p = -p_i$  in order to evaluate the coefficients of the series (A.3.3). This can also be done by the use of recurrence relations.

59. Consider the  $n \times n$  determinant  $E_{mn}$ ,  $m \leq n$ , defined in exactly the same way as  $E_{jk}$ . Then it is not difficult to show that the identities

$$E_{11} = n_0(0),$$

$$E_{mn} = n_0(0) \prod_{j=1}^{m-1} B_j, \quad m \geq 2,$$

$$E_{m,m+1} = (p + A_{m+1}) E_{mm},$$

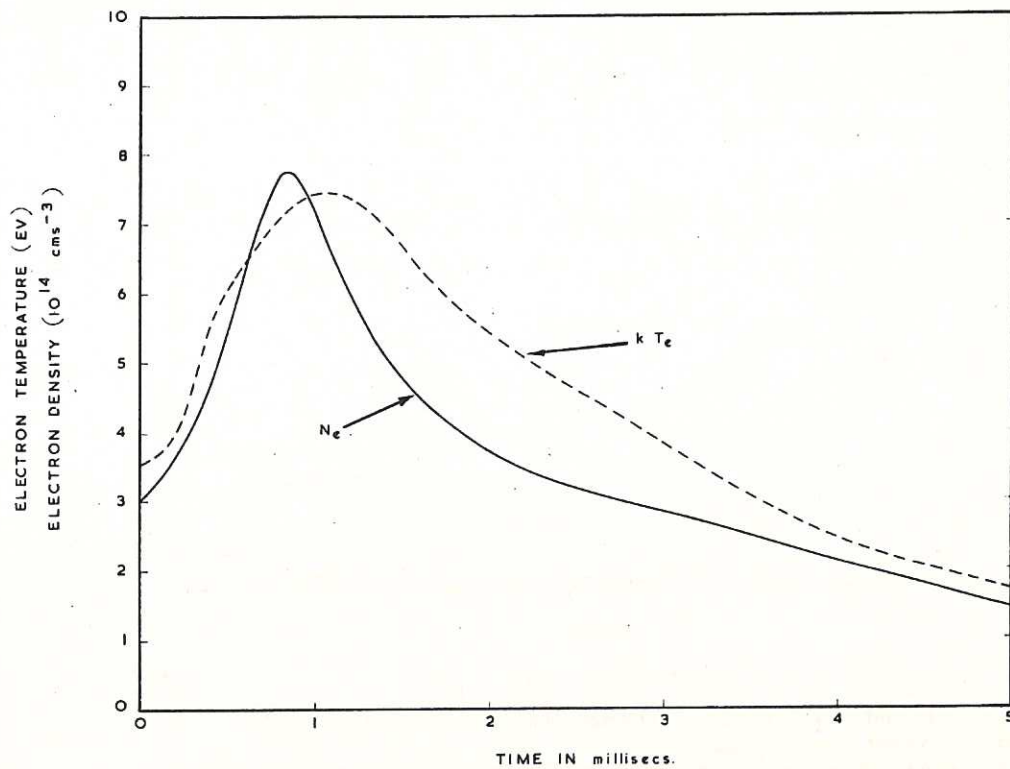
and 
$$E_{mn} = (p + A_n) E_{m,n-1} - B_{n-1} C_n E_{m,n-2}, \quad m \leq n - 2$$

are sufficient to evaluate all the  $E_{jk}$ ,  $1 \leq j \leq k$ .

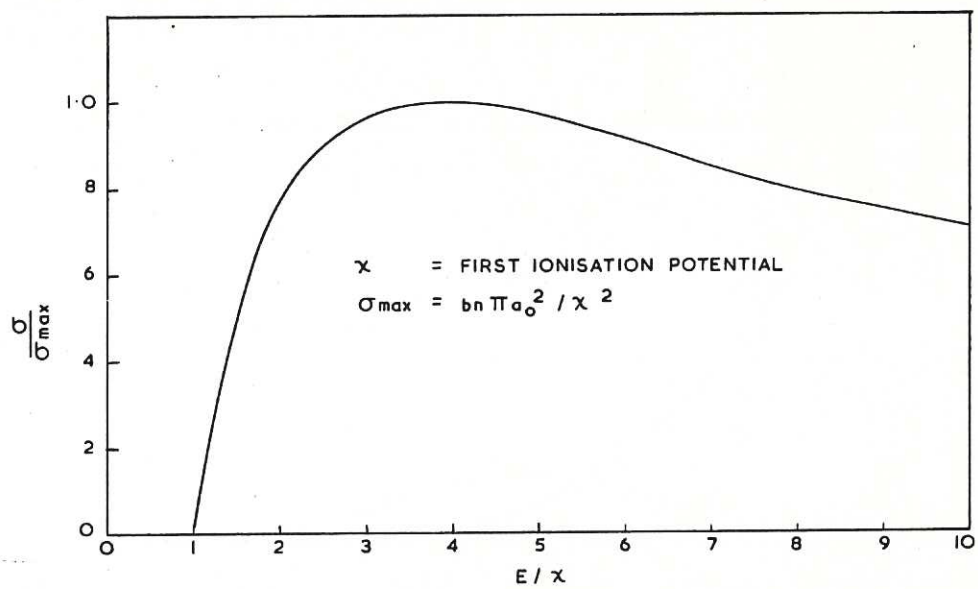
60. The methods outlined above for evaluating  $D_k^{(m)}(0)$  and  $E_{jk}(p)$  are ideally suited to programming for an automatic digital computer and provided  $k$  is not too large the method would be equally applicable to hand calculation.

## CONSTANT $n_e$

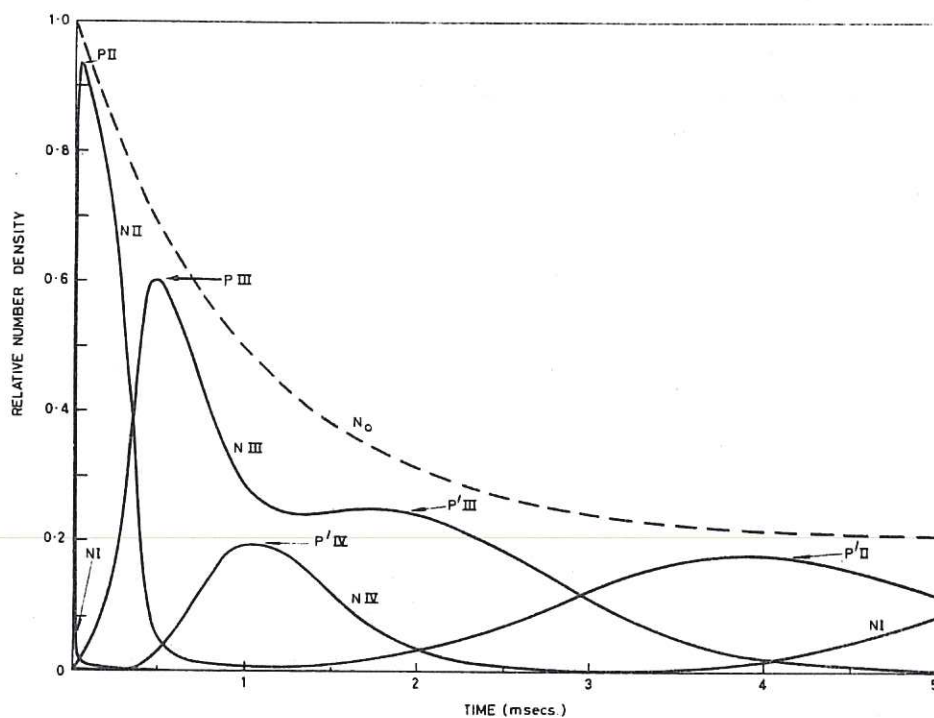
61. In the event of  $n_e$  being independent of time, i.e.  $\tau = n_e t$ , the restriction  $\lambda_i = 0$  need not be imposed. A redefinition of  $A_i$ , to the form  $A_i = S_i + \alpha_i + \lambda_i/n_e$ , would enable the calculation to proceed as before.



CLM-R 3 Fig. 1 Variation of the electron density and temperature during the discharge.

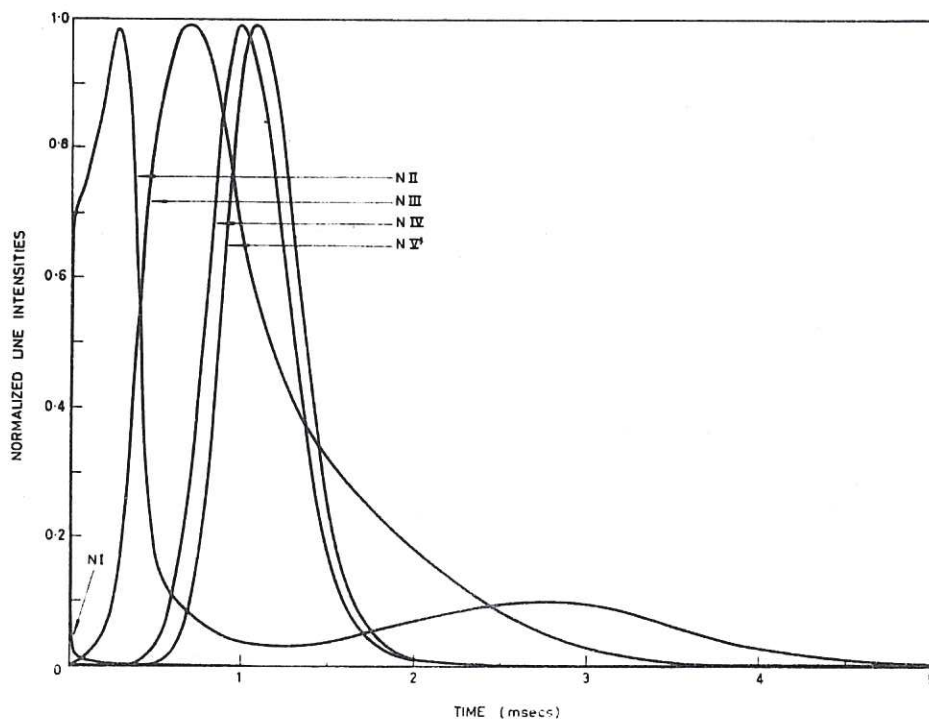


CLM-R 3 Fig. 2 Variation of ionisation cross section with energy.



CLM-R 3 Fig. 3

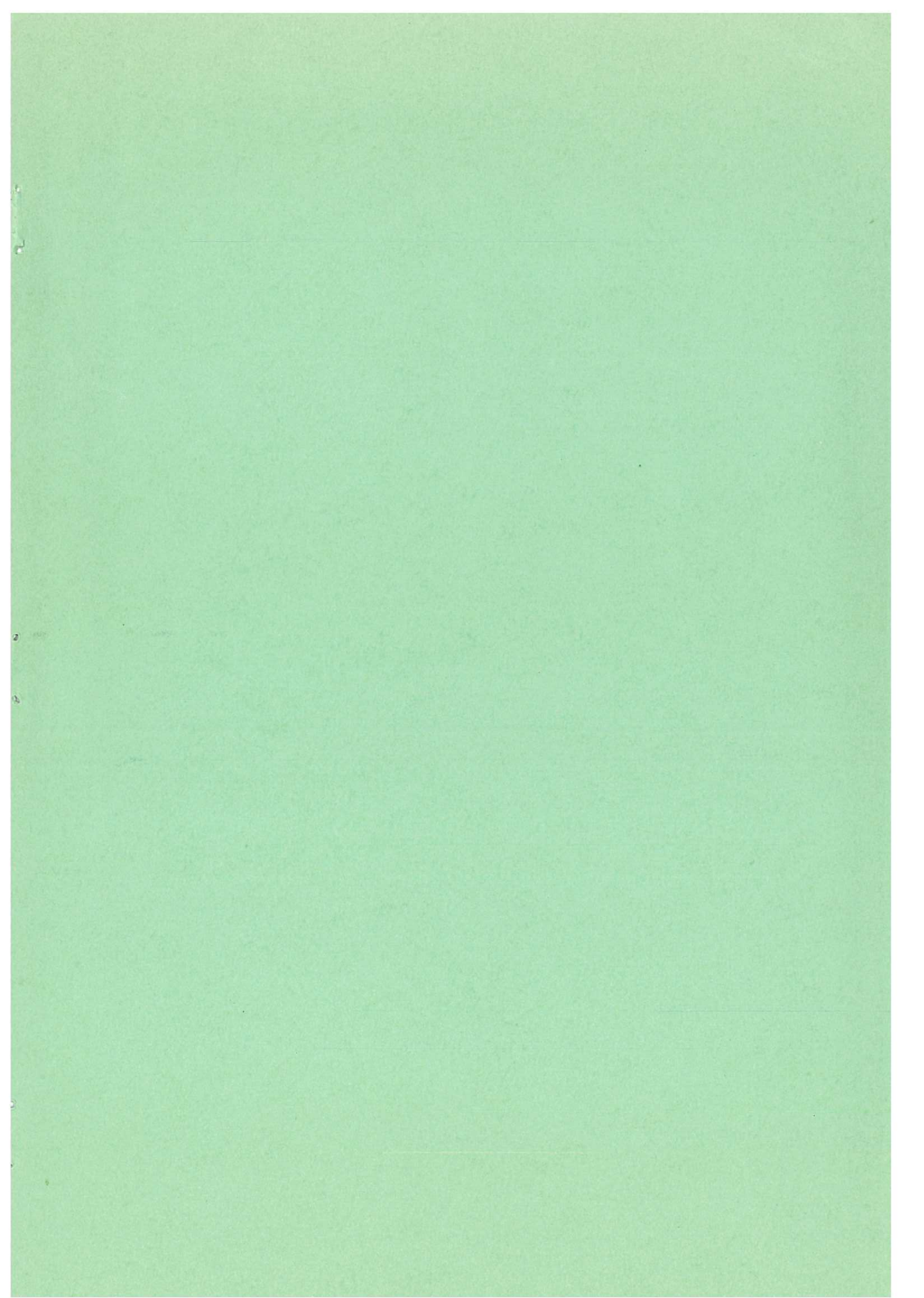
The computed variation of nitrogen ion densities (normalized to the initial number of neutrals).  
The dashed curve shows the variation of the total number of ions under the influence of loss and injection processes.



CLM-R 3 Fig. 4

The variation of nitrogen line intensities derived from the densities of Fig. 3  
The excitation potentials used were  $X_1 = 10.00$  eV,  $X_2 = 11.39$  eV,  $X_3 = 12.47$  eV,  $X_4 = 51.85$  eV and  $X_5 = 9.97$  eV.







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