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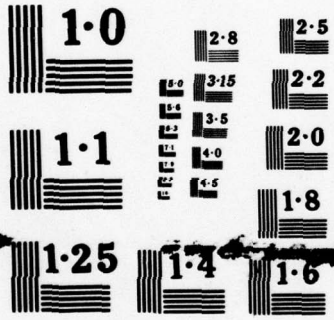

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THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES

Volume I

Theoretical Formulation of Analysis and Description of Computer Programs

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This report describes and documents a comprehensive and reasonably general computer analysis applicable to a broad class of transient, electrically excited laser systems. The theoretical model is formulated, for a spatially homogeneous medium, in terms of the coupled set of equations which describe the molecular kinetics, electron kinetics, external discharge circuit, and optical radiative extraction. One of the unique features of the present code is that the molecular kinetic subroutines for an arbitrary reaction scheme are synthesized auto-

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matically by translation of an input queue of symbolically expressed reactions into computer-coded FORTRAN equations, which are automatically coupled to a Boltzmann analysis of electron kinetics.

The molecular kinetics reaction scheme is translated into subroutines which produce the instantaneous rates $\dot{n}_i$ and the Jacobian $\delta\dot{n}_i/\delta n_j$ (for the population densities and electrical circuit parameters) so that a multistep Gear technique can be implemented for integration of the ("stiff") system of coupled equations. The radiation fields for laser extraction are formulated in terms of the intracavity photon density, with a source term from spontaneous noise and amplification (and absorption) by the excited medium. This approach allows radiation, electrons, and all of the other molecular "species" to be treated on a parallel basis.

The electron kinetics analysis consists of numerical solution of the Boltzmann equation for the electron energy distribution. The technique for solution permits inclusion of inelastic binary electron-molecule collisions, superelastic collisions, electron-electron collisions, momentum transfer (with recoil), a source term $S_0\,\delta(u) + S_b\,s(u)$ for external creation of electrons (at zero energy and over a distribution of energies) by sources of ionization, and retention of the term proportional to dn_e/dt for situations involving a net change in the electron density. From the electron energy distribution, all of the plasma parameters, electron excitation rates, and power partitioning can be obtained.

The general laser kinetics program described has been constructed with considerable emphasis on flexibility and simplicity of usage for the user. In addition to the instructions for usage described in the present report, the FORTRAN source decks contain extensive internal COMMENT card documentation as well. Even synthesized subroutines which are generated by translation of the input reaction queue contain COMMENT card documentation. In addition to the laser kinetics synthesis and analysis code, an independent program for solution of the Boltzmann equation has been developed, and is also included in the present report. All of the programs and subroutines have been written in FORTRAN IV for Extended Fortran Compilation on the CDC 6000 and CYBER Series of computers (which use a 60-bit, 10-BCD display character) word. Extensive modifications may be required if these codes are to be executed on some other system.

The present programs were developed in support of experimental research projects for the KrF excimer laser. Therefore, input and output for analysis of a KrF system are used for illustration. Program listings are given in Vol. II of this report.

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THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSES

Volume I

Theoretical Formulation of Analysis and Description of Computer Programs

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1.0 INTRODUCTION

Northrop Research and Technology Center has been involved in a variety of research programs which have resulted in significant contributions to the development of high power laser technology as well as advances in the understanding of fundamental laser physics. Recent investigations have been focused on uv and visible laser concepts, with primary emphasis on the rare gas halide excimer systems such as KrF[1-5]. In theoretical support of these experimental investigations, the present author has developed a comprehensive computer code which is sufficiently general that it would be of substantial future benefit for a wide variety of analytical studies of lasers, chemical kinetics, and electric discharge phenomena. This code*, which contains far more generality and flexibility than any of its nominal competitors currently in existence, will be thoroughly described and documented in the present report in order to make it available to the general community.

During the past several years, there has been a continuing interest and extensive effort in theoretical modeling of laser kinetic phenomena. In support of research directed toward development of new laser concepts, construction of a computer analysis to model the fundamental physical mechanisms and microscopic kinetic processes can provide a valuable tool for understanding the laser operation and for optimizing its performance. Such a model is continuously refined as understanding of the laser reaction scheme evolves.

Exploratory research for the development of promising new laser systems is often a combination of art and science, and typically requires both ex-

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* This code was developed under internal IR&D funding, with partial support from the Advanced Research Projects Agency of the Department of Defense, monitored by the Office of Naval Research under contract N00014-76-C-1100.

perimental and theoretical understanding of several overlapping disciplines such as molecular spectroscopy and kinetics, electron kinetics and discharge circuitry, fluid dynamics, and laser radiative extraction. The first step in the discovery of a new laser system is the formulation of a conceptual mechanism of excitation and energy transfer for a set of candidate atomic and molecular species; usually, this is based initially upon only an intuitive or semiquantitative understanding of the spectroscopy and kinetic processes for the proposed system. Inspiration for a concept often originates from current fundamental research in the spectroscopy of highly excited states of known molecules or unfamiliar transient species, and from studies of collision dynamics and measurements of energy transfer reaction rates. If initial experimental investigations confirm that a hypothetical laser concept can be successfully realized, more detailed studies complemented by theoretical modeling and analysis are required in order to optimize laser performance and to formulate quantitative scaling laws for extrapolation to high power, efficiency, and volume. For this purpose, it is necessary to understand the kinetic and pumping processes which are responsible for the formation and quenching of the excited species. A theoretical model of the fundamental physical mechanisms, implemented by a computer code, is a useful asset for the development and optimization of a practical laser device.

The typical development of a laser kinetic model proceeds by constructing an analysis of a spatially uniform gain medium in a simple plane parallel resonator with an attempt to describe, as completely as possible, all of the coupled phenomena involving atomic and molecular kinetics, electron kinetics, discharge circuitry, optical radiative extraction, fluid dynamics, etc. which characterize the laser system. Although the goal of such an effort is to provide a reliable analytical tool for optimizing the development of a practical laser device, such a model may also be useful even when the laser may fail to accurately exhibit the predicted

behavior in all respects. In such a case, one may still be able to define parametric trends which suggest the necessary approach for optimization of the laser device. Even with an incomplete model, it is often possible to better understand the importance of microscopic processes or excited species, and/or to eliminate some unimportant factors from further investigation. In fact, evolution in the theoretical understanding of the fundamental physical mechanisms of the laser proceeds by just such a process in which the sensitivity of various rate constants is assessed, the dependence of observed output on various experimental parameters is determined, and the kinetic reaction scheme is modified to account for and to better explain the observed phenomena. Although such a model is continually refined as the understanding of the reaction scheme evolves, even preliminary predictions from the analysis may be sufficiently reliable to justify more extensive experimental effort, or to define and narrow the range of parameters or direction of approach.

The most important theoretical components of the model consist of the analysis of the fundamental physical mechanisms, and in particular, the refinement of the molecular kinetic reaction scheme and estimates of its rate constants. Simultaneously, attempts at more sophisticated description of related problems such as discharge stability, medium nonuniformity, optical extraction and resonator configuration, flow properties, and mode-medium interactions can be undertaken. In general, all of the latter refinements are concerned more with an improved description of effects which result from spatial inhomogeneity rather than with fundamental physical mechanisms, and are therefore most appropriate only in the final stages of development of a realistic engineering model. That is not to say that these effects are unimportant, for they often present practical limitations that make it difficult to attain the results predicted for an idealized homogeneous medium.

Therefore, the scope of the present work was to develop a coupled analysis of molecular kinetics, electron kinetics, electric discharge circuit, and optical radiative extraction, which form the fundamental basis for the description of the physics of an electrically excited laser system. The goal of any such model is to successfully predict, for a spatially uniform gain medium, the excited state population densities, gain and saturation parameters, power transfer and extraction rates, electrical power partitioning, optical conversion efficiency and specific power, optical output power and spectral distribution, etc.

In general, the type of model developed, the detail and approximations considered, the computational sophistication, the input/output flexibility of the computer code, etc., can vary considerably depending upon the specific problem and application. There is currently much needless duplication of effort devoted to laser kinetic modeling. For any specific laser concept, there is often a considerable overlap as well as a frequent lack of communication between competing investigators engaged in identical kinetic analyses. Furthermore, this overlap is even more extensive when one considers the work of those who have developed essentially the same analytical models for different systems which (although not identical) are nevertheless members of a broad class of electrically excited lasers for which a more generally applicable analysis could have been developed. These concurrently developed computer codes are rarely, if ever, documented or intended for distribution. Because they vary considerably in sophistication and approach, are generally written without regard for user-orientation, often lack flexibility in problem scope or have cumbersome input/output structure, and usually require extensive effort to modify them for application to new systems, they are essentially useless to anyone but their original authors. As a result, government agencies which fund such research often pay for the same product sever-

al times, and future programs cannot directly build upon or benefit from the previous work. It is impractical to construct a new computer code for the analysis of each new kinetic reaction scheme. If the necessity of computer programming were substantially eliminated by the availability of an applicable, user-oriented, existing computer code, a significant amount of time could be saved and allocated to more productive efforts to understand the physics of the laser system.

Recognition of the lack of a coherent and unified approach to the problem of laser kinetic modeling provided the inspiration to undertake the development of a generalized computer code which would be applicable to a broad class of transient, electrically excited laser systems. The present code automatically synthesizes, for an arbitrary reaction scheme, a completely self contained computer code for numerical solution of the coupled equations which describe the molecular kinetics, electron kinetics, external driving circuit, and optical radiative extraction. This code automatically generates its own subroutines for the analysis of molecular kinetics by translating symbolic reactions, provided as input, into computer-coded equations. Thus, for the most complicated reaction scheme containing an arbitrary number of kinetic collision processes and interacting species, it is possible to obtain the complete computer code required with virtually no effort. The automatically synthesized molecular kinetics subroutines are combined with a master executive program and all other required subroutines (e.g. for numerical solution of the Boltzmann transport equation) to form a completely self-contained coupled analysis based upon the specified reaction scheme.

With appropriate modifications, this code can be easily adapted to the analysis of related problems in various fields which involve studies of chemical kinetics. Its internal subroutines for numerical solution of

the Boltzmann equation can be employed for the analysis of transport properties of electrical discharges, and a separate program developed for this purpose will be described in Sec. 3.4 (cf. Vol. II for listing).

The present computer code is completely user-oriented, and for a very broad class of transient, electrically excited laser systems, it completely eliminates the necessity for the laborious task of constructing new computer codes. It will do, automatically, work that would require several months if done manually, and it will provide an input/output flexibility for the synthesized analysis surpassing that which typically characterizes existing codes that have been developed for specific systems.

It was felt that documentation and dissemination of this computer code to those engaged in laser kinetic modeling would provide substantial benefit and economy by the elimination of needless repetition and duplication of effort. It has been the intent of the author that every effort be made to maximize the flexibility and simplicity of usage of the code, and that the description of the analysis and computational structure be sufficiently clear and detailed that others shall be able to modify and/or extend the analysis as they require. The objective has been to reduce mechanical programming considerations to a minimum, and to provide the user with (limited) diagnostic assistance as well as some protection by automatic exit if specified error conditions are encountered during execution.

The present code has been written in an extended version of FORTRAN IV with syntax and conventions compatible with the CDC 6600 computer. It makes extensive use of a 60-bit, 10-BCD character word size, as well as various special features permited by the current CDC FTN compiler, so considerable effort may be required if it should be necessary to adapt it to execute on other machines. However, because the CDC 6600 cur-

rently enjoys widespread usage for scientific applications at government, industrial, and university research laboratories, it is anticipated that the code will be suitable for the majority of potential users. In order that the program may be more easily modified or extended, the source decks have been extensively documented with internal COMMENT cards. Furthermore, even the synthesized subroutines are generated with internal COMMENT card documentation to make them completely readable and understandable. The synthesized code is a complete and self-contained FORTRAN source program.

Obviously, because this code has been developed as a research tool in support of current experimental laser development programs, it is not possible to guarantee that it will perform perfectly under all conditions to which it may be applied, although every effort has been taken to insure that it do so. Even programs which are free of logical or programming errors can fail for reasons of numerical ill-conditioning, convergence difficulties, computational instabilities, accidental division by zero, etc. Because the present code was developed primarily in support of KrF laser research, the illustrative examples to be presented in subsequent sections shall apply to that system.

It has been said that "All computer programs must be assumed to contain bugs until proven otherwise, which is impossible." Users who discover suspected "bugs" in the present analysis are encouraged to communicate them to the author who, in turn, will attempt to offer assistance to users when necessary. It is hoped that investigators who benefit from the availability of this code will make appropriate acknowledgments of its usage in the footnotes or references of their published papers, conference presentations, or reports.

2.0 SCOPE AND MATHEMATICAL STRUCTURE OF THE MODEL

The scope of the present work was the development of a comprehensive and reasonably general computer analysis applicable to a broad class of transient, electrically excited laser systems. The theoretical model is formulated, for a spatially homogeneous medium, in terms of the coupled set of equations which describe the molecular kinetics, electron kinetics, external discharge circuit, and optical radiative extraction. For each new laser kinetic scheme, the equations which define the molecular and electron kinetics are different, and the main advantage of the present computer code is that it generates the required analysis automatically by synthesizing the necessary subroutines. It is especially useful for systems characterized by complicated, but relatively unsystematic, kinetic reaction schemes. Its most appropriate application is to uv and visible laser systems which involve excitation, energy transfer, and stimulated emission from electronic states of atoms and molecules.

For infrared laser such as CO, CO_2, HF, etc., the mechanism of pumping, energy transfer, and radiative emission involves the excited vibrational levels of the ground electronic state, and for these lasers, the present approach (with modifications) would be relatively inefficient, if not totally inadequate. For the infrared laser systems, a more complicated treatment of radiation must often be included to allow for possible absorption and emission for several vibrational-rotational transitions, and there are strong temperature effects in the vibrational kinetics as well as in the radiative processes. In its present form, the analysis does not include effects of changes in the molecular temperature, and there is no provision for temperature dependent parameters. For such problems, the construction of a more specialized analysis which explicitly recognizes the systematic structure of the vibrational-rotational level interactions,

and which can most easily incorporate temperature dependent effects or other unique features, would probably be more suitable than attempts to modify, extend, and apply the present program. It is, of course, anticipated that there will be situations for which extensions or modifications of the present code, or of the subroutines which it synthesizes, will be the optimum approach.

The components of the present model, labeled with some brief descriptive remarks, are summarized in Fig. 2.1. From the more detailed discussion of the physics to be given below, it should become more apparent for which problems the present analysis is most applicable. A discussion of the limitations, approximations, numerical techniques, and range of applicability of the analysis will be provided.

2.1 Molecular Kinetics

The molecular kinetics are described by the master equation for the population densities of all the atomic and molecular species present in the electrically excited gas mixture, including electrons, ions, neutrals, excited states, excimers, etc. For a given set of reactions, the formal construction of the master equation for the population densities is illustrated in Fig. 2.2. If the species involved are $X_1, X_2, X_3, \ldots, X_n$, any reaction in the molecular kinetic scheme can be written

$$\mu_1 X_1 + \mu_2 X_2 + \mu_3 X_3 + \ldots \mu_n X_n \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \nu_1 X_1 + \nu_2 X_2 + \nu_3 X_3 + \ldots + \nu_n X_n + \Delta E \quad (1)$$

where k_f and k_r are forward and reverse rate constants (s^{-1}, cm^3/s, cm^6/s, etc.), and μ_i and ν_i are (nonnegative) integer coefficients (most of which are zero or one). The conservation of energy in Eq. (1) gives

COUPLED LASER KINETICS ANALYSIS

- MOLECULAR KINETICS

  Master Equation for population densities of all atomic and molecular species (electrons, ions, neutrals, excited states, excimers, etc.).

- ELECTRON KINETICS

  Boltzmann transport equation for the electron energy distribution to determine plasma parameters, electrical excitation rates, power partitioning, and discharge efficiency.

- CIRCUIT ANALYSIS

  External circuit equations to describe the electrical power loading in a low impedance gas discharge, whose conductivity is function of t.

- OPTICAL EXTRACTION

  Oscillator analysis, formulated in terms of intracavity photon density, with transient build-up of laser mode from spontaneous emission and subsequent relaxation to quasi-steady condition with gain at threshold.

Fig. 2.1: Basic components for the theoretical analysis of an electrically excited laser system.

MOLECULAR KINETICS

Species i: $X_1, X_2, X_3, \ldots X_i, \ldots X_n$

Reactions α:

$$\mu_1(\alpha) X_1 + \mu_2(\alpha) X_2 + \ldots + \mu_i(\alpha) X_i + \ldots$$

$$\underset{k_r}{\overset{k_f}{\rightleftharpoons}} \quad \nu_1(\alpha) X_1 + \nu_2(\alpha) X_2 + \ldots + \nu_i(\alpha) X_i + \ldots$$

Rate:

$$R(\alpha) = k_f(\alpha)[X_1]^{\mu_1(\alpha)}[X_2]^{\mu_2(\alpha)} \cdots [X_i]^{\mu_i(\alpha)} \cdots$$

$$- k_r(\alpha)[X_1]^{\nu_1(\alpha)}[X_2]^{\nu_2(\alpha)} \cdots [X_i]^{\nu_i(\alpha)} \cdots$$

Molecular Kinetics Master Equation:

$$\boxed{\frac{d[X_i]}{dt} = \sum_{\alpha} R(\alpha)[\nu_i(\alpha) - \mu_i(\alpha)]}$$

Fig. 2.3: Construction of the molecular kinetics master equation for the rates of change of population densities for an arbitrary number of interacting species in a general reaction scheme with collision processes α.

an expression for the net energy change ΔE:

$$\sum_i \mu_i E_i = \sum_i \nu_i E_i + \Delta E$$

The net rate per unit volume ($cm^{-3}s^{-1}$) R for the forward and reverse reaction of Eq. (1) is given by

$$R = k_f [X_1]^{\mu_1} [X_2]^{\mu_2} [X_3]^{\mu_3} \ldots [X_n]^{\mu_n} - k_r [X_1]^{\nu_1} [X_2]^{\nu_2} [X_3]^{\nu_3} \ldots [X_n]^{\nu_n} \quad (2)$$

where $[X_i]$ is the population density (cm^{-3}) of the i th species X_i. The contribution that such a reaction makes to the rate of production (or loss) of the i th species is given by

$$d/dt\,[X_i] = (\nu_i - \mu_i) R. \quad (3)$$

Thus, for an arbitrary reaction scheme containing several collision processes (labeled by α), the complete master equation becomes

$$d/dt\,[X_i] = \sum_\alpha [\nu_i(\alpha) - \mu_i(\alpha)] R(\alpha) \quad (4)$$

If Eq. (4) is multiplied by the energy E_i of the i th species X_i, and then summed over i, an equation for the conservation of energy (in terms of power balance) is obtained:

$$d/dt \sum_i E_i [X_i] = - \sum_\alpha R(\alpha) \Delta E(\alpha) \tag{5}$$

where

$$\Delta E(\alpha) = \sum_i [\mu_i(\alpha) - \nu_i(\alpha)] E_i \tag{6}$$

is the net energy change for reaction α. The sum over i in Eq. (5), (6) implicitly excludes secondary electrons $e^-(u)$, whose contribution to the total power conservation equation must be expressed as an integration over the continuum of electron energies u. The formulation of electrical power balance will be given in Sec. 2.3 below, where analysis of electron kinetics based upon the Boltzmann equation for the electron energy distribution is discussed. The total power balance equation will be developed in Sec. 2.5, where the physical interpretation of various terms corresponding to optical, electrical, and kinetic heating mechanisms will be given.

We may, for convenience, formally define the parameter E_i to be zero for secondary electrons, so that their exclusion from the sums in Eq. (5) and (6) does not need to be made explicit. To be consistent, it is then necessary (for the purpose of Eq. (5)) to suppress the energy dependence denoting the continuum of electron species $e^-(u)$. In doing this, it should be emphasized that the parameter $E_i = 0$ for the single species "electron" has no physical significance, and that the power balance relation (5) must ultimately be supplemented with the contributions originating from the electrical processes.

To write the subroutines which define the molecular kinetics for a complicated reaction scheme is, in general, a difficult and time-consuming

task, and the resulting computer program would have little flexibility for analysis of any system except those in a very limited class. (For example, there have been as many as ~ 80 reactions considered to be of possible importance for modeling KrF laser kinetics.) Furthermore, as understanding of a laser reaction scheme evolves, addition of new reactions (or deletion of old ones) may be continually required, in addition to making simple updated estimates of the rate constants for the reactions retained. Thus, such a code would itself have to be modified in a continuing manner, rather than merely executed with revised input values for the rate constants.

Therefore, in order to provide a more powerful analytical capability applicable to a wide class of problems, a generalized code has been developed which automatically synthesizes the coupled analysis described in Fig. 2.1 for an arbitrary reaction scheme. The input to this code is a sequence of reactions and (initial) estimates of rate constants. The syntax for the reactions is very flexible, with a free format that accepts the reaction just as it would normally be written. The content of each reaction is analyzed, and the appearance of each new species is recognized. The syntax of each reaction is subjected to numerous tests to detect errors. If the reaction is determined to be acceptable, it is decomposed and translated into appropriate computer-coded expressions in order to generate synthetically the required subroutines. Program generation and execution are protected by diagnostic assistance and automatic exit (according to input requests) if specified error conditions are encountered. A more detailed discussion of the structure of the code will be given in a subsequent section devoted specifically to program description.

Fig. 2.3 presents a schematic flow diagram of the present approach. The rate constants initially assumed in the generation of the program

can be changed in the subsequent execution, if desired. The main purpose of the rate constants in the initial input deck is to define whether the forward and/or reverse process is to be included in the rate expressions. If, during program generation, a zero rate constant is encountered for any process (other than secondary electron collisions), no translation of the forward (or backward) term occurs in the synthesized subroutines. Of course, if the correct values of the rate constants are known, they may be entered for once and for all in the original input deck. As Fig. 2.3 indicates, the synthesized molecular kinetics subroutines are automatically combined with the master executive program and all other required subroutines to form a completely self-contained coupled analysis based upon the specified reaction scheme. The section enclosed in the upper box in Fig. 2.3 is required only when a new reaction scheme is introduced and generation of a new program is required. For all subsequent calculations based upon the given reaction scheme, the initial conditions, experimental parameters, rate modifications (if any), and I/O and control parameters are entered, and the complete code constructed in the upper box is executed. That is, only the lower section of Fig. 2.3 is involved thereafter.

There are several obvious advantages to this approach. First of all, there is the simplicity of automation and the minimization of the possibility of error in the writing of complicated subroutines. Secondly, the program diagnoses error conditions in the reaction syntax which may not have been noticeable or which may have been overlooked. For example, duplicate reactions are detected (even when written backwards), charge particle and heavy particle conservation is insured, detail balance relations for binary collision processes are enforced, and miscellaneous other error conditions are detected. Secondary electron collision processes are recognized and properly coupled to the electron kine-

GENERALIZED SYNTHESIS LASER KINETICS CODE

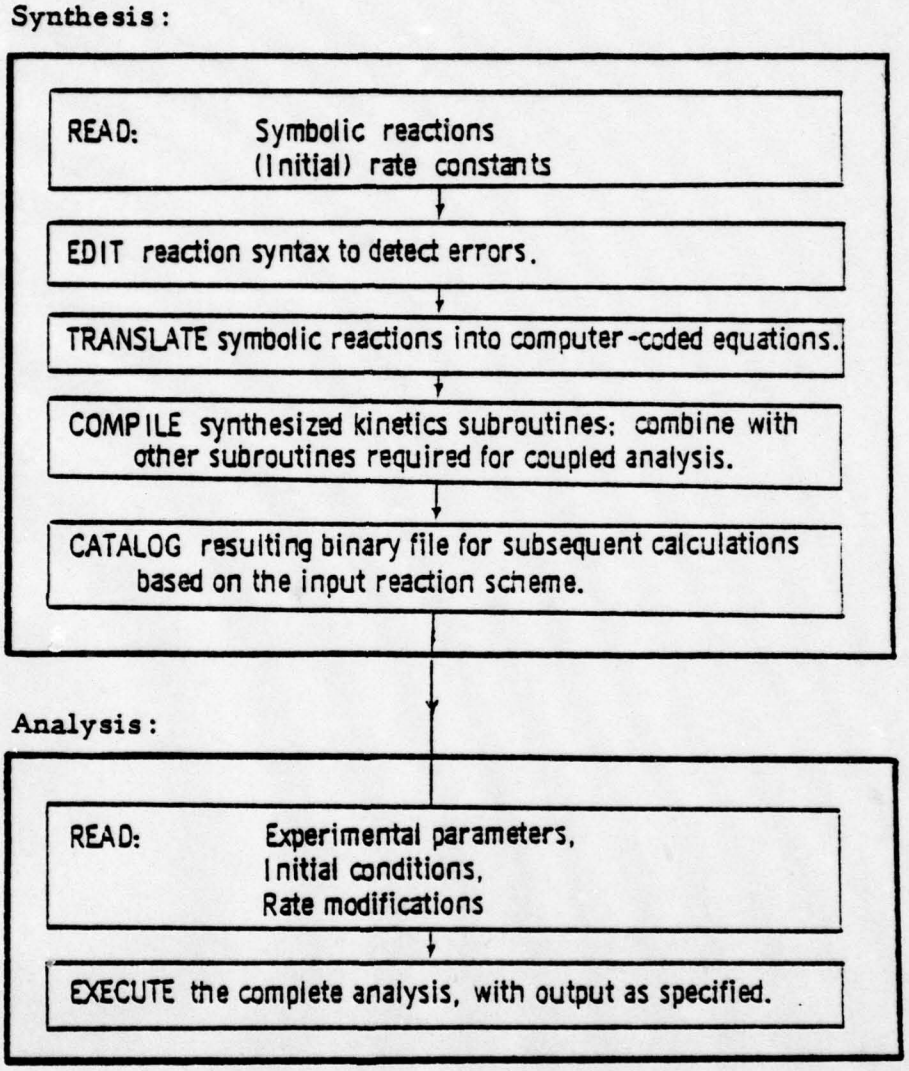


Fig. 2.3: Schematic flow diagram of the functional structure of the laser kinetics code. A complete FORTRAN source program is synthesized by translation of symbolic reactions into computer-coded equations. Execution of the analysis occurs in the lower box.

tics analysis, except for cases without electric discharge (e.g. e^--beam excitation only), in which case their rate constants can be defined by input. Finally, the subroutines are constructed in such a way that null operations (multiplications or additions involving zero) are completely eliminated (if no rate constant is provided for the forward or reverse process, no translation of the corresponding term occurs), and in such a way as to optimize computational efficiency (repetitious or unnecessary multiplications are minimized). Even for relatively simple problems with uncomplicated molecular kinetic reaction schemes, the availability of a program which can automatically provide the investigator with a user-oriented code with good I/O flexibility and simplicity of usage is of obvious advantage.

It is usually the case that the rate constants involved in molecular kinetic reaction schemes can vary over several orders of magnitude, and therefore, the resulting master equation (4) often becomes a "stiff" system of differential equations. Therefore, the approach which has been taken for integration of these equations is to employ a multistep technique developed by Gear[6]. This method automatically adjusts the integration step size as the solution proceeds, in such a way that required accuracy conditions are maintained. The Gear method requires subroutines not only for the rates of change $\dot{n}_i = d[X_i]/dt$ of the population densities, but also for the Jacobian, $\delta \dot{n}_i / \delta n_j$, as a function of time. Because numerical evaluation of the Jacobian is not generally satisfactory, it is necessary to generate both such subroutines symbolically in the synthesis section of the program, where the reaction scheme is decomposed and translated into computer-coded equations.

The entry of control parameters, experimental parameters, revised rate constants, initial conditions, output requests, etc., is quite flexible, and

permits the code to be executed for a variety of situations of interest. For example, rate constants for secondary electron collisions are obtained self-consistently from the coupled Boltzmann analysis for the case of an electric discharge. For the case of e^--beam excitation only, these rate constants default automatically to zero, but can be specified by input, if desired. This is useful for entering thermal (i.e. room temperature) values for electron recombination or attachment processes, for example. Thus, the same general code can be used for both discharge or e^--beam excitation conditions. Likewise, it is possible to apply it to either an oscillator or amplifier analysis.

The integration of the coupled set of equations over the total specified pulse length is carried out with the Gear technique, which automatically adjusts the step size to maintain accuracy and stability. However, the total pulse length is divided into a finite number (nominally 50) of subintervals, at which time the electron kinetics are updated and a variety of output option requests can be supplied.

2.2 Radiative Extraction

The basic features of the radiation analysis are summarized in Fig. 2.4. Because considerable simplification can be achieved by neglecting complications associated with a rigorous description of the optical fields in a realistic resonator configuration, a spatially homogeneous medium is assumed, with an optical resonator formed by two plane parallel mirrors. The net amplification of the intracavity radiation intensity $I(\nu)$ from the stimulated emission and absorption process

$$X^* + I(\nu) \underset{}{\overset{\sigma}{\rightleftharpoons}} X + I(\nu), \qquad (7)$$

OPTICAL EXTRACTION

- Spatially uniform intracavity optical fields.
- Plane parallel optical resonator (100%, R), separation L_c.
- Spatially uniform gain medium of length L_g.
- Distributed output coupling and loss (Y) coefficients.
- Cavity threshhold gain coefficient:

$$\alpha_{th} = [Y + (1/2)\ln(1/R)]/L_g$$

- Buildup of optical fields:

  Spontaneous emission in solid angle Ω defined by output coupling aperture and resonator length: A/L_c^2.

  Amplification from stimulated emission, offset by the intracavity absorption and output coupling losses.

- Formulation in terms of intracavity photon density:

$$n_{ph} = I/ch\nu$$

$$dn_{ph}(t)/dt = (L_g/L_c)\left[c[\alpha(t) - \alpha_{th}]\, n_{ph}(t) + \frac{N^*}{\tau}\frac{\Omega}{4\pi}\right]$$

- Cavity buildup time: $t_c = L_c/L_g\alpha_{th}c$

Fig. 2.4: Basic formulation of radiative extraction in terms of intracavity photon number density, with buildup of optical fields from spontaneous emission.

corresponding to the laser transition from an excited state X^* to a lower state X, as well as by absorption processes such as

$$A + I(\nu) \xrightarrow{\sigma_{abs}(A)} A^* \tag{8}$$

can be written

$$dI(t)/dt = c[\alpha(t) - \alpha_{th}]I(t), \tag{9}$$

where $\alpha(t)$ is the instantaneous net gain coefficient in the medium (i.e. active gain offset by absorption),

$$\alpha(t) = [N^*(t) - N(t)]\sigma - \sum_A n_A(t)\sigma_{abs}(A), \tag{10}$$

and α_{th} is the cavity threshold loss coefficient. Actually, (9) applies only to the situation where the cavity length L_c and the gain gength L_g of the active medium are equal; if they are unequal, it must be modified to read

$$dI(t)/dt = (L_g/L_c)c[\alpha(t) - \alpha_{th}]I(t) \tag{11}$$

The factor L_g/L_c has the significance of a contraction in the radiative time scale to account for the fact that during a round trip cavity time, the gain medium is encountered during only a fraction (L_g/L_c) of that time. Equivalently, if the gain medium were considered to be distributed uniformly over the entire cavity length L_c (rather than over the actual gain length L_g), then the actual gain would have to be reduced by the factor L_g/L_c to produce an equivalent round trip amplification. It should also be noted that L_g/L_c is the ratio of the active gain volume to the optical cavity volume, and therefore this factor logically appears in the formulation of the equation for conservation of power density.

It is convenient to treat stimulated emission and absorption processes in a manner parallel to that for kinetic collision reactions. Therefore, the equation for radiative extraction will be formulated in terms of the photon number density in the cavity, defined by

$$n_{ph} = I/ch\nu. \tag{12}$$

This will also facilitate the incorporation of spontaneous emission as a source term for the buildup of the optical fields from noise. The equation for the photon number density includes the source term from spontaneous emission, amplification from stimulated emission, and losses from output coupling and/or intracavity absorption:

$$dn_{ph}/dt = (L_g/L_c)\left[N^*/\tau(\Omega/4\pi) + c\left[\alpha(t) - \alpha_{th}\right]n_{ph}\right]. \tag{13}$$

$\alpha_{th} = \left[\gamma + (1/2)\ln(1/R)\right]/L_g$ is the threshold loss coefficient expressed in terms of the intracavity loss per pass γ and the output coupling reflectivity R, $(\Omega/4\pi)$ is the fractional part of the total spontaneous emission which builds up the laser mode (taken to be the solid angle Ω subtended by the output coupling mirror viewed from the opposite end of the cavity), and $\alpha(t)$ is the instantaneous net gain coefficient in the medium defined by Eq. (10).

Note that transient effects are included in the present description of the radiation field. Although a steady state oscillation condition (i.e., for which the gain and loss coefficients are equal) will typically occur during the time scales of interest, such a condition is not an a priori assumption of the present analysis. This approach allows the radiation intensity to be described for situations where pumping and kinetic times are comparable to the cavity decay time,

$$t_c = L_c/(L_g c \alpha_{th}). \tag{14}$$

For such situations, gain relaxation effects can be observed in which the net gain initially overshoots the cavity threshold and subsequently decays to the steady state gain condition, $\alpha(t) = \alpha_{th}$. Under conditions of high pumping the overshoot can be significant, since the stimulated emission from the medium occurs under conditions of high gain.

When formulated in terms of the intracavity photon density, the radiation equations can be included in a unified way with the other kinetic collision processes of the laser reaction scheme. For example, the stimulated emission process (7) can be described by the equations

$$dN^*/dt = -k_f N^* n_{ph} + k_r N n_{ph} = k(N - N^*) n_{ph} \tag{15.1}$$

$$dN/dt = -dN^*/dt \tag{15.2}$$

$$dn_{ph}/dt = (L_g/L_c) k (N^* - N) n_{ph}, \tag{15.3}$$

where $k_f = k_r = k = c\sigma$, and σ = stimulated emission (and absorption) cross section (cm^2). Likewise, the contribution of reaction (8) to the photon field is

$$dn_{ph}/dt = -(L_g/L_c) k_{abs}(A) n_A(t) n_{ph}, \tag{16}$$

where $k_{abs}(A) = c\,\sigma_{abs}(A)$ is the rate constant for absorption (cm^3/s). Although minor modifications are required to incorporate the factors $(\Omega/4\pi)$ and (L_g/L_c) and the term $-c\,\alpha_{th} n_{ph}$ in Eq.(13), the similarity in structure of Eq. (3), (15), and (16) permits the radiation field (photons) to be treated on an equal basis with the other molecular species in the construction of the master equation described earlier.

2.3 Electron Kinetics: Boltzmann Equation

The present analysis of an electrically excited laser medium incorporates a completely coupled treatment of molecular and electron kinetics. The electron kinetics analysis is based upon the assumption that the plasma has attained a quasisteady state on the time scales of electrical pumping and inelastic secondary electron collision processes, so that the electron energy distribution function f(u) can be obtained from solution of the time-independent Boltzmann equation as a function of gas mixture and the instantaneous values of E/N and excited state population densities. The present analysis includes electron-molecule inelastic collisions, elastic electron-molecule momentum transfer collisions (with recoil), electron-electron (i.e., Coulomb) scattering, and excitation from an applied (dc) electric field as well as source terms for electron creation (and resulting energy deposition) from an external e^--beam. Superelastic electron collisions (i.e., reverse processes in which electrons gain energy by collisions with excited molecular species) are important in situations with high excited state population densities, and are included in both the molecular and plasma kinetic equations. Electron-electron scattering effects, which can become important under conditions of high fractional ionization, are included. From the solution of the Boltzmann equation, all of the electron transport coefficients, elastic and inelastic secondary electron collision rates, electrical power partitioning, etc., can be obtained.

One of the unique features of the present analysis is a self-consistent treatment of secondary ionization and attachment phenomena by retention of a quasisteady term proportional to dn_e/dt to properly account for transient plasma effects that occur on the time scale of the molecular and electron kinetic processes. The usual formulation of the time-

ELECTRON KINETICS ANALYSIS

- Electron Energy Distribution $f_0(u)$: Numerical solution of the Boltzmann transport equation.

- Quasisteady state approximation: the term proportional to dn_e/dt is retained to describe situations for which there is a net creation (or loss) of electrons.

- Source term included to describe external ionization (e.g., electron beam or photoionization):

$$S(u) = S_0 \delta(u) + S_b(u).$$

  S_0 term provides for the external creation of electrons at zero energy.

- Momentum transfer with recoil; elastic heating of the molecular gas.

- Binary inelastic electron-molecule collision processes included; e.g.,

  Vibrational Excitation, Electronic Excitation, Secondary Ionization, Attachment, Recombination, Dissociation, etc.

- Electrons created by secondary ionization assumed to be at zero energy and included in a source term $\sim \nu_i \delta(u)$.

- Electron-electron collisions (Coulomb scattering) are included (important for high fractional ionization, $\gtrsim 10^{-5}$).

- Charged particle interactions between electrons and heavy ions neglected.

- Superelastic collisions, important for excited gas mixtures, are included.

- Electrical parameters, calculated as a function of E/N, gas mixture, and the excited state population densities:

  Mobility, Drift Velocity, Average Energy, Effective Temperature, Characteristic Energy, Diffusion Coefficient, Plasma Conductivity, Discharge Current Density, Power Densities.

  Forward (and reverse) secondary electron excitation rates.

  Fractional partitioning of electrical input power into rate of energy storage and all elastic and inelastic scattering mechanisms.

Fig. 2.5: Summary of features of the electron kinetics analysis.

independent Boltzmann equation assumes that the inelastic processes include only binary electron-molecule collisions for which there is no net creation or loss of secondary electrons. When creation or loss of electrons occurs by secondary ionization, attachment, recombination, external sources of ionization, etc., it is necessary to retain the term proportional to dn_e/dt in the time-dependent Boltzmann equation in order to properly describe the conservation of electron density. If the electron energy distribution f(u) were known, the rates of secondary ionization, attachment, recombination, etc. could all be calculated and dn_e/dt could be determined. However, dn_e/dt occurs as a parameter in the Boltzmann equation, and in order to calculate f(u), its value must be known. Therefore, an iterative approach was developed for a self-consistent determination of dn_e/dt. The numerical techniques for solution of the Boltzmann equation will be described in detail later.

The basic features of the electron kinetics analysis are summarized in Fig. 2.5. The scope of the present analysis is considered to be quite comprehensive. In addition to the fact that the present formulation includes more refinements than many of the Boltzmann analyses currently in usage, the computer subroutine for its numerical implementation is quite flexible and computationally efficient.

Theoretical Formulation

In general, the electron energy distribution function for the gas mixtures and relatively low E/N values typical of electric discharge lasers is highly non-Maxwellian. The increasing availability of extensive experimental cross section data for elastic and inelastic electron collision processes for many gases of interest often makes it possible to obtain a quantitative analysis of electron kinetics by direct numerical solution of the Boltzmann equation. If there is no net creation or loss of electrons by external source, secondary ionization, recombination, or at-

tachment, the electron velocity distribution $f(\vec{v})$ for a multicomponent gas in an external electric field $\vec{E}(\vec{r}, t)$ satisfies the Boltzmann transport equation,

$$\left[\partial/\partial t + \vec{v}\cdot\vec{\nabla}_{\vec{r}} - (e/m)\vec{E}(\vec{r}, t)\cdot\vec{\nabla}_{\vec{v}}\right] f(\vec{v}, \vec{r}, t) = \delta f/\delta t \Big|_c \qquad (17)$$

where the collision term on the right hand side includes the effects of all elastic and inelastic scattering processes. A detailed discussion of the Boltzmann transport equation can be found in works by Holstein[7], Allis[8], Schkarofsky et al[9], Frost and Phelps[10], Carleton and Megill[11], and Englehardt et al[12, 13]. Various approximations and techniques for its numerical solution and application to the analysis of electric discharge gas lasers have been discussed by Nighan et al[14], Rockwood[15], Hancock et al[16], Elliott et al[17], Morgan and Fisher[18], Lowke et al[19], Lacina[20], and others. The present approach is based upon extensions and generalizations of earlier work[20] related to analysis of CO kinetics.

At the gas densities of interest for laser operation, elastic and inelastic electron-molecule collision frequencies are so high, relative to those for molecular kinetic processes, that the electron distribution function can be assumed to have adjusted "instantaneously" on the time scales over which the excited state population densities are evolving. It follows, therefore, that the first term of Eq. (17) containing the partial time derivative can be discarded if the electric field $\vec{E}(\vec{r}, t)$ is assumed to be dc or slowly varying. For a spatially uniform field, it is similarly possible to neglect the second term, since the mean free path (which is related to the elastic collision cross section and molecular density) is typically small compared to the discharge dimensions. Thus, the Boltzmann equation (17) becomes

$$-(e/m)\vec{E}\cdot\vec{\nabla}_{\vec{v}} f(\vec{v}) = \delta f/\delta t \Big|_c . \qquad (18)$$

The usual approach for solving this equation begins with an expansion of $f(\vec{v})$ into Legendre polynomials,

$$f(\vec{v}) = f_o(v) + (\vec{v}/v)\cdot\vec{f}_1(v) + [3\vec{v}\vec{v}/v^2 - \tilde{1}]:\tilde{f}_2(v) + \ldots \qquad (19)$$

($\tilde{1}$ and $\tilde{f}_2$ represent dyadic quantities.) Usually, f can be well approximated using only the first two terms,

$$f(\vec{v}) = f_o(v) + (\vec{v}/v)\cdot\vec{f}_1(v). \qquad (20)$$

Physically, the justification of a two-term approximation is related to assumptions about the degree of anisotropy to be expected for the velocity distribution. If the electric field is small enough that the directed speed of the electrons (as measured by their drift velocity) is much less than their random thermal velocities, the small first order perturbation $\hat{v}\cdot\vec{f}_1$ from an isotropic distribution $f_o(v)$ should be a good approximation. For high values of E/N characteristic of self-sustained discharges and for certain gases, it has been speculated[21] that the $\tilde{f}_2$ term may be comparable to the $\vec{f}_1$ term, although no analysis has yet been undertaken to include these higher order terms quantitatively. Retention of more than the first two terms would require knowledge of angular (i.e. differential scattering) cross section data, which is not generally available. Typical experimental data gives only integrated cross sections (over all angles) as a function of the electron energy. Some of the available data in the literature has been determined indirectly by fitting measured transport coefficients to synthetic cross sections, using a numerical Boltzmann analysis based upon the two-term expansion (20) of $f(\vec{v})$. Thus, consistent use of that data would require that the electron kinetics calculations be based upon the two-term approximation. For values of E/N typical of e^--beam sustained discharges, this approach is justified, and it is numerically much simpler than would be the case if angular calculations were required.

In the expansion (19), $f_o(v)$, $\vec{f}_1(v)$, $\tilde{f}_2(v)$, ... are functions only of the magnitude $v = |\vec{v}|$, since all of the angular dependence has been put explicitly into the spherical harmonic coefficients $\hat{v}$, $(3\hat{v}\hat{v} - \tilde{1})$, ... etc. It can easily be verified that

$$\nabla_v f(\vec{v}) = \frac{1}{3v^2}(d/dv)(v^2\vec{f}_1) + (df_o/dv)\hat{v} + (v/3)(d/dv)(v\vec{f}_1)\cdot (3\hat{v}\hat{v} - \tilde{1}) + \ldots \tag{21}$$

where $\nabla_v f(\vec{v})$ has been separated into spherical harmonic terms which have $\ell = 0, 1, 2$ symmetry, respectively. If (21) is substituted into (18) and separated into scalar and vector parts (which corresponds to multiplying by 1 or $\hat{v}$ and integrating over the spherical solid angle Ω_v), the following equations result:

$$-(e\vec{E}/3mv^2)\cdot(d/dv)(v^2\vec{f}_1) = \delta f_o/\delta t\Big|_c \tag{22.1}$$

$$-(e\vec{E}/m)(df_o/dv) = \delta\vec{f}_1/\delta t\Big|_c \tag{22.2}$$

The most important physical mechanism for reducing the asymmetry in the distribution function is electron-molecule momentum transfer collisions. The collisional rate of change of $\vec{f}_1$ can be approximated by[9]

$$\delta\vec{f}_1/\delta t\Big|_c = -\sum_X \nu_m^X(v)\,\vec{f}_1, \tag{23}$$

where $\nu_m^X(v) = N_X v Q_m^X(v)$ is the momentum transfer collision frequency for molecules X in terms of the population density N_X and momentum transfer cross section $Q_m^X(v)$. In terms of the electron energy

$$u = mv^2/2e \tag{24}$$

(with u in units of eV, $e = 1.602\ 10^{-12}$ erg/eV $= 1.602\ 10^{-19}$ J/eV), the

equation for $f_o(u)$ becomes, after manipulation of Eq. (22) and (23),

$$- (E^2/3)\, d/du \left[\frac{u}{\sum_X N_X Q_m^X(u)} df_o(u)/du \right] = \frac{mv}{2e} \frac{\delta f_o}{\delta t}\bigg|_c . \qquad (25)$$

Expressions for the collision term $\delta f_o/\delta t\big|_c$ on the right hand side of Eq. (25) have been derived by Holstein[7], Allis[8], Schkarofsky et al[9], Frost and Phelps[10], and numerous others. It shall not be the purpose of the present discussion to repeat these extensive and rigorous derivations here.

However, it may be useful at least to motivate the form of the results for inelastic binary collisions characterized by an isotropic scattering cross section. For an inelastic scattering process, the collision term is defined simply as the net flux of electrons scattered into, and out of, a region $[\vec{v}, \vec{v} + \Delta\vec{v}]$ of velocity space. The electrons scattered into $[\vec{v}, \vec{v} + \Delta\vec{v}]$ originate from all volume elements $[\vec{v}', \vec{v}' + \Delta\vec{v}']$ for which energy is conserved:

$$(1/2)\, mv'^2 = (1/2)\, mv^2 + e u_o \qquad (26.1)$$

or,

$$u' = u + u_o, \qquad (26.2)$$

where u_o is the inelastic energy loss (eV) for the scattering process, and Eq. (24) was used. Under the assumption of isotropic scattering, Eq. (26) uniquely defines $\Delta\vec{v}'$ for an arbitrary choice of $\vec{v}$ and $\Delta\vec{v}$, for we can set $\Delta\vec{v} \sim v^2 \Delta v$, $\Delta\vec{v}' \sim v'^2 \Delta v'$, and invoke Eq. (26) to obtain $\Delta v'/\Delta v = v/v'$. Therefore, it follows that

$$\Delta\vec{v}' = (v'/v)\Delta\vec{v}. \tag{27}$$

The rate ($cm^{-3}s^{-1}$) at which electrons are scattered out of $[\vec{v}', \vec{v}'+\Delta\vec{v}']$ is given by $f(\vec{v}')\Delta\vec{v}' N v' Q(v')$, where $Q(v')$ is the scattering cross section and N is the neutral molecule particle density. Recall that $f(\vec{v}')\Delta\vec{v}'$ represents the spatial density of electrons (cm^{-3}) in the velocity region $[\vec{v}', \vec{v}'+\Delta\vec{v}']$, and that $N v' Q(v')$ has the significance of collision frequency (s^{-1}). In order to obtain an expression for the total flux of electrons scattered into $[\vec{v}, \vec{v}+\Delta\vec{v}]$ from $[\vec{v}', \vec{v}'+\Delta\vec{v}']$, it is necessary to sum the contributions from all velocities $\vec{v}'$ which satisfy the conservation of energy condition. The required "sum" over the continuum of velocities $\vec{v}'$, restricted by Eq. (26), can be expressed as an integral over $d\vec{v}'$, weighted by a density function

$$F(u') = \delta(u' - u - u_o) \Big/ \int d\vec{v}''\, \delta(u'' - u - u_o).$$

It is easy to show that $F(u')\,d\vec{v}' = du'\,\delta(u' - u - u_o)$, and therefore the restricted "sum" over velocities $\vec{v}'$ is equivalent to integration over all energies u' weighted by the distribution $\delta(u' - u - u_o)$. Thus, the collision term can be written

$$\Delta\vec{v}\ \delta f(\vec{v})/\delta t\Big|_c = -f(\vec{v})\Delta\vec{v}\, v\, N\, Q(v)$$

$$+ \int du'\,\delta(u' - u - u_o)\, f(\vec{v}')\Delta\vec{v}'\, v'\, N\, Q(v'),$$

where the first term represents scattering out of (and the second term scattering into) the region $[\vec{v}, \vec{v}+\Delta\vec{v}]$ of velocity space. From Eq. (27) it follows that the collision term can be expressed as

$$\delta f(\vec{v})/\delta t\Big|_c = (N/v)\left[f(\vec{v}')\,v'^2\,Q(v')\Big|_{v'^2 = v^2 + 2eu_o/m} - f(\vec{v})\,v^2\,Q(v)\right] \quad (28)$$

To lowest order in the expansion (20), $f(\vec{v}) = f_o(v)$ depends only upon the magnitude v, as is the case for Q (v), and therefore all quantities can be expressed as functions of the energy u. Thus, the lowest order inelastic collision term becomes

$$\delta f_o(u)/\delta t\Big|_c^{in} = \frac{2e}{mv} N\left[(u+u_o)f_o(u+u_o)Q(u+u_o) - u f_o(u)\,Q(u)\right], \quad (29)$$

where Eq. (24) and (28) have been used. For all collision processes (both elastic and inelastic), there will be a contribution to $\delta f_o/\delta t\Big|_c$ originating from momentum transfer. (Whenever an electron of energy u undergoes a collision process with a neutral molecule of mass M, there is a transfer of energy of order $\sim (m/M)\,u$ resulting from momentum conservation.) The momentum transfer contribution is[7-10]:

$$\delta f_o(u)/\delta t\Big|_c^{el} = \frac{2e}{mv}(d/du)\left[u^2 \sum_X \frac{2m}{M_X} N_X Q_m^X(u)\left(f_o + \frac{kT}{e}\frac{df_o}{du}\right)\right] \quad (30)$$

Combining Eq. (25), (29), and (30), we obtain the following form for the Boltzmann equation:

$$(E^2/3)\,d/du\left[u\,df_o/du/\langle NQ_m\rangle\right] + d/du\left[u^2\langle(2m/M)NQ_m\rangle\left(f_o + \frac{kT}{e}\frac{df_o}{du}\right)\right]$$

$$+ \sum_\alpha \Big[(u+u_\alpha)f_o(u+u_\alpha)N_\alpha Q_\alpha(u+u_\alpha) - u f_o(u) N_\alpha Q_\alpha(u)$$

$$+ (u-u_\alpha)f_o(u-u_\alpha)N_\alpha^* Q_{-\alpha}(u-u_\alpha) - u f_o(u) N_\alpha^* Q_{-\alpha}(u)\Big] = 0 \quad (31)$$

where $Q_{\pm\alpha}(u)$ are the (forward and reverse) cross sections for the inelastic collision processes, labeled by α, N_α and N_α^* are the population densities of the lower and upper (excited) states, and u_α is the inelastic energy loss associated with the collision. The two weighted averages which occur in Eq. (31) are defined by

$$\langle N Q_m(u) \rangle = \sum_X N_X Q_m^X(u), \tag{32.1}$$

$$\langle (2m/M) N Q_m(u) \rangle = \sum_X (2m/M_X) N_X Q_m^X(u) \tag{32.2}$$

The principle of detailed balance provides relations between the cross sections $Q_{\pm\alpha}(u)$ for the forward and reverse (superelastic) processes:

$$(u + u_\alpha) Q_\alpha(u + u_\alpha) = u Q_{-\alpha}(u) \tag{33.1}$$

$$(u - u_\alpha) Q_{-\alpha}(u - u_\alpha) = u Q_\alpha(u) \tag{33.2}$$

The first two terms in the sum over α in Eq. (31) correspond to collisions in which the electrons lose energy, while the last two terms (which represent the superelastic processes) correspond to collisions in which excited molecular species transfer their energy to the electrons. Only binary electron-molecule collisions, including vibrational excitation, electronic state excitation, attachment, recombination, ionization, etc. will be considered. It should be emphasized, however, that the formulation of the Boltzmann equation as given by Eq. (31) applies only to a quasisteady state situation for which there is no net creation or loss of electrons. If processes such as secondary ionization, electron attachment or recombination are included, Eq. (31) is valid only under condi-

tions for which the collision frequencies for such processes are much lower than those for the inelastic excitation processes which do not involve the creation or loss of electrons. It should be noted that the collision term for such inelastic processes does not contain all four of the terms indicated in the general expression given in Eq. (31). For example, only the second term occurs for recombination or attachment (in which an electron is lost), and for ionization or dissociation, only the first two terms occur (since there is no reverse binary collision process). Because of the low density of states available for momentum conservation, two-body recombination is generally a very slow process. Electron recombination proceeds as a three-body process, which cannot be treated according to the present formulation. However, it is often found experimentally that the rates for three-body recombination vary with pressure as if the process were two-body, and thus, effective cross sections can be used to describe it as a binary collision appropriate for the formulation of Eq. (31). Thus, for (schematic) processes such as

Attachment: $A + e^- \rightarrow B^- + C$ (34.1)

Two-Body Recombination: $A^+ + e^- \rightarrow B + C$ (34.2)

the inelastic collision term in Eq. (31) consists only of

$$- u f_o(u) N_\alpha Q_\alpha(u). \tag{35}$$

For processes such as

Secondary Ionization: $B + e^- \rightarrow B^+ + e^- + e^-$ (36.1)

Dissociation: $AB + e^- \rightarrow A + B + e^-$ (36.2)

the collision term contains only

$$(u+u_\alpha) f_o(u+u_\alpha) N_\alpha Q_\alpha(u+u_\alpha) - u f_o(u) N_\alpha Q_\alpha(u). \tag{37}$$

Furthermore, in the case of secondary ionization, there is the creation of an additional electron. Because experimental knowledge of ionization cross sections is not usually available in the detail necessary to describe the final energy distribution of the created electrons, it is often assumed that the additional electrons are created at zero energy, and that they relax into the distribution on the same time scale (given by the elastic collision frequency) over which the rapid attainment of a quasisteady state occurs. Therefore, the collision term for secondary ionization requires an additional modification, the inclusion of a term

$$\delta(u) N_\alpha \int_o^\infty du\, u f_o(u) Q_\alpha(u). \tag{38}$$

Perhaps a more realistic hypothesis would be to assume that the final electrons have equal energies or, better still, that their energies are partitioned according to a purely kinematic distribution of a three-body breakup. It is believed that such assumptions, which needlessly complicate the analysis, would provide no additional physical insight. Therefore, the electrons created by secondary ionization are assumed to have zero energy.

The effects of recoil in momentum transfer collisions are included in the second term of Eq. (31), where the molecular energy distribution has been assumed to be Maxwellian at temperature T. Note that, if there is no electric field and if kT is much less than the energy thresholds for the inelastic collision processes, then an approximate solution for the electron energy distribution is obtained by equating the

second term of Eq. (31) to zero, giving

$$f_o(u) = \exp\left[-eu/kT\right].$$

This is to be expected, since electrons and molecules would be in thermal equilibrium with each other in that case. The momentum transfer term in Eq. (31) is important for low values of E/N at low temperatures, and for gas mixtures containing light molecules. The physical significance of that term is elastic heating of the molecular gas, to be discussed in more detail in Sec. 2.5. The higher the value of the lowest inelastic excitation threshold, the more important will be the fractional power partition into elastic heating for a given value of E/N. For molecular gases, characterized by vibrational level excitation processes with very low energy thresholds (typically $\sim 0.1 - 0.2$ eV), elastic heating is negligible for values of E/N characteristic of typical laser excitation ($\gtrsim 3 \times 10^{-17}$ Vcm^2). However, for rare gas laser mixtures for which the lowest inelastic energy loss usually corresponds to excitation of an electronic level ($\sim$ few eV), the contribution of elastic heating can be significant even for relatively high values of E/N (e.g. $\sim 10^{-16}$ Vcm^2). Effects of rotational excitation, which are not included in the present version of the electron kinetics analysis, can be incorporated[9, 10] into the Boltzmann equation in the same way as momentum transfer by making a suitable continuum approximation.

Most authors have not only restricted their attention to solution of the Boltzmann equation in the form of Eq. (31), but have often ignored the superelastic collision terms. For weakly excited gases, such an approach is justified, providing that attachment and secondary ionization could be neglected. However, in order to properly describe effects of interest in electrically excited lasers, superelastic collisions must be

included, and in addition, several important extensions to the formulation (31) of the Boltzmann equation are necessary.

First of all, the contribution (38), representing the creation of electrons (at zero energy) from secondary ionization, must be included in the collision term of Eq. (31).

Secondly, it is useful to incorporate a source term $S_{ext}(u)$ to describe (as a function of energy) the creation of electrons by external sources of ionization (e.g., e^--beam, photoionization, etc.) and the resulting energy deposition. Since there are often several electron creation processes for which no a priori knowledge of this energy dependence is available (e.g., Penning ionization, photodetachment, photoionization by intracavity radiation), it is convenient to assume that the resulting electron energy is zero. Thus, the source term is assumed to be of the form

$$S_{ext}(u) = S_o \delta(u) + S(u), \tag{39}$$

where S_o represents a rate ($cm^{-3}s^{-1}$) of creation of electrons at zero energy, and $S(u)$ represents a rate of creation per unit energy ($cm^{-3}s^{-1}$ eV^{-1}) of electrons of energy u (i.e., $S(u)du$ is the rate of creation of electrons in the energy interval $[u, u+du]$). The first term, which can be used to include all electron creation processes arising from excited-state interactions in the medium, contributes nothing to energy deposition into the electron gas (since the electrons have zero energy). The second term $S(u)$ is used to describe electron creation from an external source, typically e^--beam ionization. A more detailed discussion of energy (power) balance is given in Sec. 2.5.

Third, in order to properly conserve electron number density, a term proportional to dn_e/dt must be retained from the time-dependent Boltzmann equation. The term $\partial n_e(u,t)/\partial t$ (where $n_e(u,t)\,du = n_e(t)\,du\,u^{1/2} f_o(u)$ is the electron density in the energy interval $[u, u+du]$) can be written

$$\partial n_e(u,t)/\partial t = u^{1/2} f_o(u,t)\, dn_e/dt + n_e(t)\, u^{1/2}\, \partial f_o(u,t)/\partial t. \qquad (40)$$

It is reasonable to retain the earlier assumption that the <u>shape</u> $f_o(u,t)$ is not an explicit function of the time, since a quasisteady state will be established on a time scale much shorter than that characteristic of molecular and electron kinetic processes. Thus, $f_o(u)$ will be only an implicit function of time through its dependence upon instantaneous values of various parameters, such as E/N, and the excited state population densities $N_\alpha(t)$. It follows that the second term in Eq. (40) can be deleted, and the explicit time dependence in $f_o(u,t)$ suppressed in the first term. The first term must be retained, even in the quasisteady state approximation, since it represents the net rate of creation (or loss) of electrons on the time scale of attachment, recombination, ionization, etc. It will be shown that retention of the dn_e/dt term is necessary to insure that the first integral of the Boltzmann equation correctly results in the conservation equation for the electron number density $n_e(t)$. Since dn_e/dt occurs as a parameter whose value cannot be determined until the equation is solved, a self-consistent iterative method (to be discussed in more detail later) was developed.

Finally, the effects of Coulomb scattering can become important[15, 21]

under conditions of high fractional ionization, so electron-electron collisions must be included. (Charged particle interactions between electrons and heavy ions will be neglected in the present analysis.) For a highly ionized gas, electron-electron collisions dominate electron-molecule collisions, and this tends to force the electron energy distribution to become more nearly Maxwellian. Rockwood[15] has shown how the Boltzmann equation can be expressed in terms of a "flux divergent" description of the electron distribution in energy space, and how electron-electron collisions can be incorporated into such a formulation.

Accounting for these refinements, the Boltzmann equation becomes

$$u^{1/2} f_o(u)\, dn_e/dt + dJ_f(u)/du + dJ_{el}(u)/du + dJ_{ee}(u)/du =$$

$$S_o\, \delta(u) + S(u) + n_e \sqrt{\frac{2e}{m}} \left\{ \delta(u) \sum_i N_i \int_o^\infty du\, u\, f_o(u)\, Q_i(u) + \right.$$

$$\sum_\alpha \Big[(u+u_\alpha) f_o(u+u_\alpha) N_\alpha Q_\alpha(u+u_\alpha) - u f_o(u) N_\alpha Q_\alpha(u)$$

$$\left. + (u-u_\alpha) f_o(u-u_\alpha) N_\alpha^* Q_{-\alpha}(u-u_\alpha) - u f_o(u) N_\alpha^* Q_{-\alpha}(u) \Big] \right\}. \qquad (41)$$

The sum over i represents a sum over all secondary ionization processes. The sum over α corresponds to the complete set of all inelastic electron-molecule collisions, including ionization, with the tacit understanding (according to the foregoing discussion) that certain terms in the general collision expression are to be omitted for processes for which there is a net creation or loss of electrons, or for which there is no reverse binary collision. (I. e., the collision term is reduced to the expressions (35) or (37) in such cases.) The "current densities" $J_f(u)$,

$J_{el}(u)$, and $J_{ee}(u)$, which correspond to a flux of electrons in energy space driven by the applied electric field, elastic scattering collisions, and electron-electron collisions, are defined by

$$J_f(u) = -(E^2/3)\, n_e \sqrt{\frac{2e}{m}}\, [\, u\, df_o/du \big/ \langle N Q_m(u) \rangle] \tag{42.1}$$

$$J_{el}(u) = -n_e \sqrt{\frac{2e}{m}}\, u^2 \langle (2m/M) N Q_m(u) \rangle [f_o + \frac{kT}{e}\frac{df_o}{du}] \tag{42.2}$$

$$J_{ee}(u) = -(2\pi/3)\, n_e^2 \sqrt{\frac{2e}{m}} (q^4/e^2) \ln\Lambda\, [\, P(u)\frac{df_o}{du} + Q(u) f_o] \tag{42.3}$$

where

$$P(u) = 2\int_o^u dw\, w^{3/2} f_o(w) + 2u^{3/2}\int_u^\infty dw\, f_o(w), \tag{43.1}$$

$$Q(u) = 3\int_o^u dw\, w^{1/2} f_o(w). \tag{43.2}$$

In the above equations, $q = 300\,e = 4.8 \times 10^{-10}$ esu is the electronic charge (cgs units), $e = 1.602 \times 10^{-12}$ erg/eV, and Λ is the ratio of the Debye length ℓ_D and the classical distance of closest approach r_o (for an electron of average energy $u = \bar{u}$), defined by

$$\Lambda = {}_D/r_o \tag{44}$$

$$\ell_D = (kT_e/4\pi n_e^2)^{1/2} \tag{45}$$

$$r_o = q^2/(e\bar{u}) = 2q^2/3kT_e. \tag{46}$$

Comparison of Eq. (31) with Eq. (41) shows that they are equivalent, except for the inclusion of the additional terms dn_e/dt for electron conservation, $S(u)$ for external ionization sources, $dJ_{ee}(u)/du$ for electron-electron collisions, and the term $\sim\delta(u)$ representing the creation of electrons (at zero energy) by secondary ionization and the external source S_o. The formulation (41) of the Boltzmann equation to be used in the present analysis is written in such a way that its significance as a continuity equation (in energy space) is manifestly apparent. In Fig. 2.6, an interval $[u, u + du]$ of energy space is depicted, with an electron "current density" $J(u)$. If there is an external source $S_{ext}(u)$ and a (non-local) source $S_{coll}(u)$ from inelastic collisions driving electrons into (and out of) the interval $[u, u + du]$, the continuity equation can be written

$$du\left[dn_e(u,t)/dt\right] + \left[J(u+du) - J(u)\right] = du\left[S_{ext}(u) + S_{coll}(u)\right]$$

or,

$$dn_e(u,t)/dt + dJ(u)/du = S_{tot}(u) \tag{47}$$

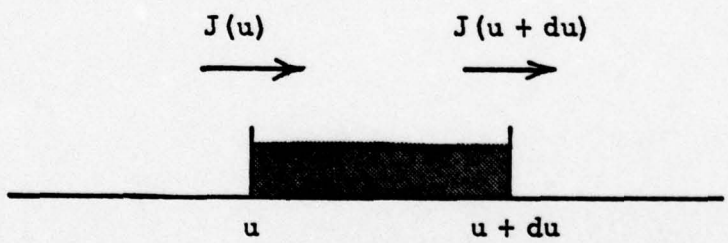


Fig. 2.6: Continuity equation interval.

Thus, the first term on the left hand side of Eq. (41) represents the rate of change of electron density in the interval $[u, u+du]$, while the dJ/du terms represent electron flux in energy space driven by the applied electric field, elastic collisions, and electron-electron scattering. On the right hand side of (41), there are source terms from ex-

ternal ionization, secondary ionization, and nonlocal inelastic scattering of electrons into and out of the interval $[u, u+du]$.

The normalization condition for $f_o(u)$ is taken to be

$$\int_o^\infty du\, u^{1/2} f_o(u) = 1, \tag{48}$$

where the factor $u^{1/2}$ originates from the density of states associated with the transformation from the three-dimensional velocity space $\vec{v}$ to the energy space u: $d\vec{v} = 4\pi v^2 dv = 2\pi(2e/m)^{3/2} u^{1/2} du$. (Thus, the units of $f_o(u)$ will be $eV^{-3/2}$.) From the solution $f_o(u)$ of the Boltzmann equation (41), all of the forward and reverse electron excitation rates $\langle v Q_{\pm\alpha}(u) \rangle$, electrical power partitioning, and miscellaneous plasma parameters (drift velocity v_d, mobility μ, average and characteristic energies $\bar{u}$ and ϵ_k, effective temperature T_e, etc.) can be obtained:

Collision Rates (cm^3/s):

$$\langle v Q_{\pm\alpha}(u) \rangle = (2e/m)^{1/2} \int_o^\infty du\, u\, f_o(u)\, Q_{\pm\alpha}(u) \tag{49}$$

Mobility (cm^2/Vs):

$$\mu = -(1/3)(2e/m)^{1/2} \int_o^\infty du\, [u/\langle N Q_m(u) \rangle]\, df_o/du \tag{50}$$

Diffusion Coefficient (cm^2/s):

$$D = (1/3)(2e/m)^{1/2} \int_o^\infty du\, [u/\langle N Q_m(u) \rangle]\, f_o(u) \tag{51}$$

Average Energy (eV):

$$\bar{u} = \int_o^\infty du\, u^{3/2} f_o(u) \tag{52}$$

Effective Temperature (K):

$$T_e = (2/3)\bar{u}/k \tag{53}$$

Characteristic Energy (eV):

$$\epsilon_k = D/\mu \tag{54}$$

Drift Velocity (cm/s):

$$v_d = \mu E \tag{55}$$

For the case of an ac electric and/or applied magnetic fields, there are other transport coefficients of interest, and expressions for these quantities as well as discussion of the extensions of the Boltzmann equation required to describe these phenomena can be found in the references[8-10].

The first integral (from 0 to ∞) of Eq. (41) gives an expression for the conservation of electron density:

$$dn_e/dt = n_e[\nu_i - \nu_a] + \int_0^\infty du\, S(u) + S_o, \tag{56}$$

where

$$\nu_i = \sum_i N_i \langle v Q_i(u) \rangle \tag{57}$$

and

$$\nu_a = \sum_a N_a \langle v Q_a(u) \rangle \tag{58}$$

are the total secondary ionization and electron attachment frequencies. Note that for all of the inelastic scattering processes which conserve

electrons, the integral over the collision term vanishes:

$$\int_0^\infty du \left[(u+u_\alpha) f_o(u+u_\alpha) Q_\alpha(u+u_\alpha) - u f_o(u) Q_\alpha(u) \right] = 0, \quad (59)$$

which can be shown by shifting the variable of integration and noting that $Q_\alpha(u) = 0$ for $u < u_\alpha$. For attachment or recombination, however, only the term (35) occurs in the collision expression, leaving the ν_a term in Eq. (56). For secondary ionization, both terms shown in Eq. (59) appear and the integral vanishes; however, there is still a term in Eq. (56) containing ν_i originating from the $\delta(u)$ term in Eq. (41). The integral of $S(u)$ on the right hand side represents the total rate of change of electron density from the external source.

It is apparent that the term proportional to dn_e/dt must be retained in order to correctly obtain conservation of electron density in situations where creation or loss of electrons is important. Obviously, this will always be the case for transient analysis of pulsed electrical lasers if it is important to properly describe the build-up of the plasma. Note that Eq. (31), which does not include the dn_e/dt term, may give rise to solutions for $f_o(u)$ which contain logarithmic singularities at $u = 0$. To demonstrate this, consider the case of attachment only, and integrate the Boltzmann equation from u to ∞:

$$J(\infty) - J(u) = - n_e \nu_a$$

As $u \to 0$, (since $J(\infty) = 0$), this becomes an equation of the form

$$[A u^2 + B u] \, df_o/du = n_e \nu_a$$

which is characterized by a singularity at $u = 0$.

If Eq. (41) is multiplied by eu and integrated over all energy, an expression for electrical power balance is obtained:

$$e n_e \mu E^2 + \int_0^\infty du\,(eu)\,S(u) = e\bar{u}\,dn_e/dt +$$

$$n_e\, e(2e/m)^{1/2} \left\{ \int_0^\infty du\, u^2 \langle (2m/M)\, N\, Q_m \rangle \left[f_o + (kT/e) df_o/du \right] \right.$$

$$\left. + \sum_\alpha u_\alpha \int_0^\infty du\, u\, f_o(u) \left[N_\alpha Q_\alpha(u) - N_\alpha^* Q_{-\alpha}(u) \right] \right\} \qquad (60)$$

The form of the inelastic collision term on the RHS of Eq. (60) results from a change of variables in the first term of an expression, such as

$$N_\alpha \left\{ \int_0^\infty du\, u(u+u_\alpha)\, f_o(u+u_\alpha)\, Q_\alpha(u+u_\alpha) - \int_0^\infty du\, u^2 f_o(u)\, Q_\alpha(u) \right\}$$

$$= N_\alpha \int_0^\infty du\, f_o(u)\, Q_\alpha(u) \left[u(u-u_\alpha) - u^2 \right]$$

$$= -N_\alpha u_\alpha \int_0^\infty du\, u\, f_o(u)\, Q_\alpha(u) \qquad (61)$$

Note that, for processes such as ("two-body") electron recombination and attachment (in which an electron is lost), only the second term of the form (35) (i.e., $-u f_o(u) N_\alpha Q_\alpha(u)$) occurs in Eq. (41). In that case, the first term on the LHS of Eq. (61) is absent and the corresponding term in the power balance equation (60) must be modified:

$$N_\alpha \int_0^\infty du\, u^2 f_o(u)\, Q_\alpha(u) \qquad (62)$$

The physical interpretation of Eq. (60) is that the total electrical input power density (discharge and external deposition) on the left hand side is partitioned into $e\bar{u}\,dn_e/dt$ (representing the rate of change of electron

kinetic energy stored in the electron gas), elastic heating from momentum transfer collisions, and dissipation by the inelastic excitation processes on the right hand side. Note that the contribution from electron-electron scattering vanishes--this mechanism merely redistributes the electron energy and tends to drive the distribution toward a Maxwellian shape. To show that the electron-electron contribution vanishes, integrate by parts,

$$\int_0^\infty du\, u\, dJ_{ee}(u)/du = J_{ee}(u)\Big|_0^\infty - \int_0^\infty du\, J_{ee}(u), \tag{63}$$

and the first term on the right vanishes because $P(\infty) = 2\bar{u}$, $Q(\infty) = 3$, $P(0) = Q(0) = 0$, and $f_o(\infty) = df_o(\infty)/du = 0$. Thus,

$$-\int_0^\infty du\, u\, dJ_{ee}(u)/du = \int_0^\infty du\, J_{ee}(u)$$

$$= -(2\pi/3)\, n_e^2 (q^4/e^2) \ln\Lambda \int_0^\infty du \left[P\, df_o/du + Q f_o(u)\right](2e/m)^{1/2}$$

Suppressing the constant factor, and integrating the first term by parts gives

$$\int_0^\infty du \left[P\, df_o/du + Q f_o\right] = P(u) f_o(u)\Big|_0^\infty + \int_0^\infty du\, f_o \left[Q - dP/du\right]$$

$$= \int_0^\infty du\, f_o(u) \left[Q(u) - dP/du\right] \tag{64}$$

From the definitions (43),

$$Q(u) - dP(u)/du = 3\left\{ \int_0^u dw\, w^{1/2} f_o(w) - u^{1/2} \int_u^\infty dw\, f_o(w) \right\} \tag{65}$$

and the expression in (64) becomes

$$\int_0^\infty du\, f_o(u)\left[Q(u) - dP(u)/du\right] =$$

$$3\left\{\int_0^\infty du\, f_o(u)\int_0^u dw\, w^{1/2} f_o(w) - \int_0^\infty du\, u^{1/2} f_o(u)\int_u^\infty dw\, f_o(w)\right\}$$

Interchanging the variables (u, w) in the second term above gives

$$\int_0^\infty du\, f_o(u)\left[Q(u) - dP(u)/du\right] =$$

$$3\left\{\int_0^\infty\int_0^u - \int_0^\infty\int_w^\infty\right\} du\, dw\, w^{1/2} f_o(u) f_o(w) = 0 \qquad (66)$$

Since both of the integrals in Eq. (66) are carried out over the same (infinite) 45° sector in the upper half of the (u, w) plane defined by $0 \le u < \infty$, $0 \le w \le u$, the electron-electron contribution vanishes.

From the definition of inelastic collision rate given by (49), the power balance equation (60) can be written, finally, as

$$e n_e \mu E^2 + e\langle U^+\rangle S_b = e\bar{u}\, dn_e/dt +$$

$$e n_e (2e/m)^{1/2} \int_0^\infty du\, u^2 \langle (2m/M) N Q_m\rangle \left[f_o + (kT/e)\, df_o/du\right]$$

$$+ n_e \sum_\alpha{}' (eu_\alpha)\left[N_\alpha \langle v Q_\alpha(u)\rangle - N_\alpha^* \langle v Q_{-\alpha}(u)\rangle\right]$$

$$+ n_e e (2e/m)^{1/2} \sum_a N_a \int_0^\infty du\, u^2 f_o(u) Q_a(u) \qquad (67)$$

where the sum over "a" is over all attachment and recombination pro-

cesses, which are to be implicitly excluded from the sum over all the other inelastic collisions α. S_b is the total rate of creation of electrons with positive energies,

$$S_b = \int_0^\infty du\, S(u) \tag{68}$$

and an average deposition energy $\langle U^+ \rangle$ has been defined as a weighted average of the external ionization source function $S(u)$ as

$$\langle U^+ \rangle = \int_0^\infty du\, u\, S(u) \Big/ \int_0^\infty du\, S(u). \tag{69}$$

The typical source of external ionization is a high energy electron beam. The mathematical description of the energy deposition in the gas is, in general, quite complicated and several investigators have developed extensive computer programs for such analysis. It is beyond the scope of the present work to describe the physics of e^--beam ionization, so it is not possible to indicate how the form of the excitation source function $S(u)$ is determined. If the origin of the source ionization is an external e^--beam of current density J_b (A/cm^2), then the function $S(u)$ could be expressed in terms of cross sections $\sigma_i^+(u)$ as

$$S(u) = (J_b/e) \sum_i \sigma_i^+(u)\, N_i\,, \tag{70}$$

where the sum is over all species i ionized by the beam. The total deposition of e^--beam energy associated with ionization is then

$$e\langle U^+ \rangle S_b = \langle U^+ \rangle \sum_i \sigma_i^+ N_i J_b = J_b\, dV^+/dx, \tag{71}$$

where $\sigma_i^+ = \int du\, \sigma_i^+(u)$, and an effective voltage drop has been defined as $dV^+/dx = \langle U^+ \rangle / \ell$ in terms of a "mean free path" ℓ for ionization,

$$\ell^{-1} = \sum_i \sigma_i^+ N_i. \tag{72}$$

A similar term dV^*/dx occurs for e^--beam deposition corresponding to excited states.

Numerical Approach

The numerical solution of the Boltzmann equation (41) is carried out by reducing the differential equation to a finite difference equation, defined over a uniform grid of equally spaced energy values ($0 = u_1, u_2, u_3, \ldots \ldots u_M = u_{max}$), where the maximum energy u_{max} satisfies, typically, $u_{max} \gtrsim 5\bar{u}$. This results in a large set of coupled algebraic equations (typically $M > 500$) which could be solved (at least formally) by a matrix inversion. However, a straightforward matrix inversion is not practical computationally or from the standpoint of computer core storage that would be required. For example, a typical energy range of (0, 20) eV, subdivided into a mesh of $M = 500$ to give an energy resolution of 0.04 eV, would require storage and manipulation of 500 x 500 matrices, each of which would contain $250,000 \approx 1,000,000_8$ elements. To reduce the problem of core storage and matrix inversion, an iterative approach that utilizes the advantages of sparse matrices (i.e. matrices whose elements are mostly zeros) has been developed. The essence of the present technique[16] is the reduction of the system of linear difference equations to a form which involves the inversion of only tridiagonal matrices, for which computation time and core storage are substantially reduced.

With some recent exceptions, most of the work which has been done to

implement the numerical solution of the Boltzmann equation has been associated with problems for which the excited state population densities are negligible, and for which the superelastic collision terms can therefore be omitted. In that case, electrons always lose energy in collisions, and for any given energy u the inelastic collision term on the right hand side of (41) involves only $f_o(u)$ and $f_o(u + u_\alpha)$--i.e. the values for the distribution function f_o evaluated at energies equal to and greater than u. Therefore, one of the most common approaches to the numerical solution of the Boltzmann equation has been to assume a fixed value for $f_o(u_{max})$, integrate (41) backward from $u = u_{max}$ to $u = 0$, and finally to impose the normalization condition (48). If the superelastic terms are retained, then terms containing $f_o(u - u_\alpha)$ occur, and the backward integration scheme fails. Attempts to extend this technique to the superelastic case have generally encountered difficulties and limited success.

Under highly excited conditions typical of laser plasmas ($N^*/N \gtrsim 10^{-5}$), superelastic collision terms must be retained. Their inclusion presents no difficulties for the present technique, which is based upon an iterative solution of the set of linear difference equations obtained from (41) and reduced to tridiagonal form. The algorithm developed is extremely fast, and execution speed is optimized when a good initial guess for f_o is available. Thus, the present approach is especially suitable for a coupled analysis in which the excited state population densities and discharge voltage change as a function of time, since the previous electron distribution (at some time t) provides a good initial guess for obtaining the updated distribution (at time $t + \Delta t$). As an example: for an electron grid of 500 points, with 15 inelastic collision processes and electron-electron scattering, the electron distribution function f_o converged to an accuracy $< 2 \times 10^{-3}$ after ~ 8 iterations in ~ 0.7 CF sec-

onds on the CDC 6600 computer (from an initial guess for $f_o(u)$ given by $e^{-eu/kT}$, for example). The numerical techniques for the solution of Eq. (41) will be described in detail below.

The functional values of the distribution $f_o(u)$ defined over the uniform grid of energy values ($0 = u_1, u_2, u_3, \ldots, u_M = u_{max}$) shown in Fig. 2.7 will be denoted by ($f_1, f_2, f_3, \ldots, f_M$), and the spacing of the energy grid will be denoted by Δu:

$$
\begin{aligned}
M &= MESH + 1 \\
\Delta u &= u_{max}/MESH \\
u_i &= (i - 1)\Delta u \\
f_i &= f_o(u_i)
\end{aligned}
\tag{73}
$$

where $i = 1, 2, 3, \ldots, M$.

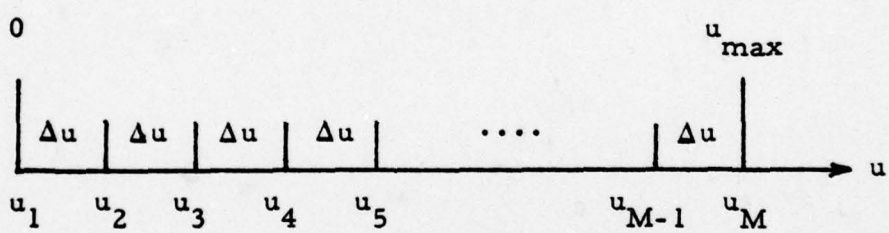


Fig. 2.7: Uniform energy grid.

If Eq. (41) is integrated from $(u_i - \Delta u/2)$ to $(u_i + \Delta u/2)$ for $i = 2, 3, 4, \ldots, M$, with the tacit boundary condition that $f_{M+1} = 0$, the result is a system of $(M - 1)$ coupled algebraic equations:

$$\left\{ J_f(u) + J_{el}(u) + J_{ee}(u) \right\} \Bigg|_{u_i - \Delta u/2}^{u_i + \Delta u/2} + dn_e/dt \int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du\, u^{1/2} f_o(u) =$$

$$\int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du \left[S(u) + (n_e \nu_i + S_o)\delta(u) \right] +$$

$$n_e \sqrt{\frac{2e}{m}} \sum_\alpha \int_{u_i - \Delta u/2}^{u_i + \Delta u/2} du \Big[(u + u_\alpha) f_o(u + u_\alpha) N_\alpha Q_\alpha(u + u_\alpha) - u f_o(u) N_\alpha Q_\alpha(u)$$

$$+ (u - u_\alpha) f_o(u - u_\alpha) N_\alpha^* Q_{-\alpha}(u - u_\alpha) - u f_o(u) N_\alpha^* Q_{-\alpha}(u) \Big] \qquad (74)$$

All of the integrals which occur in Eq. (74) will be approximated by the values of the integrand taken at the midpoint u_i. The values of f_o and df_o/du which occur in Eq. (74) at the midpoint energies,

$$u_i^{\pm} = u_i \pm \Delta u/2 \qquad (75)$$

are approximated by

$$f_o(u_i \pm \Delta u/2) = f_o(u_i^{\pm}) = (f_{i\pm 1} + f_i)/2 \qquad (76.1)$$

$$f_o'(u_i \pm \Delta u/2) = f_o'(u_i^{\pm}) = \pm (f_{i\pm 1} - f_i)/\Delta u. \qquad (76.2)$$

For convenience, we define the following functions:

$$p(u) = (E^2/3)\, u / \langle N Q_m(u) \rangle + (kT/e)\, u^2 \langle (2m/M) N Q_m(u) \rangle$$

$$+ (2\pi/3)(q^4/e^2)\, n_e \ln\Lambda\, P(u) \qquad (77)$$

$$q(u) = u^2 \langle (2m/M) N Q_m(u) \rangle + (2\pi/3)(q^4/e^2)\, n_e \ln\Lambda\, Q(u) \qquad (78)$$

in terms of which the total "current density" can be expressed as

$$J(u) = J_f(u) + J_{el}(u) + J_{ee}(u)$$

$$= - n_e (2e/m)^{1/2} \left[p(u) \frac{df_o}{du} + q(u) f_o(u) \right] \qquad (79)$$

With the above definitions and approximations, Eq. (74) becomes

$$- p(u_i^+)(f_{i+1} - f_i)/\Delta u + p(u_i^-)(f_i - f_{i-1})/\Delta u - q(u_i^+)(f_{i+1} + f_i)/2$$

$$+ q(u_i^-)(f_i + f_{i-1})/2 + (2e/m)^{-1/2} \Delta u \left[\frac{\dot{n}_e}{n_e} u_i^{1/2} f_i - \frac{S_i}{n_e} - \delta_{i,2} (\nu_i + \frac{S_o}{n_e}) / \Delta u \right.$$

$$= \Delta u \sum_\alpha \left[(u_i + u_\alpha) f_o(u_i + u_\alpha) N_\alpha Q_\alpha (u_i + u_\alpha) - u_i f_i N_\alpha Q_\alpha (u_i) \right.$$

$$\left. + (u_i - u_\alpha) f_o(u_i - u_\alpha) N_\alpha^* Q_{-\alpha}(u_i - u_\alpha) - u_i f_i N_\alpha^* Q_{-\alpha}(u_i) \right] \qquad (80)$$

where $S_i = S(u_i)$. For convenience, define the quantities

$$p_i^\pm = p(u_i^\pm) = p(u_i \pm \Delta u/2)$$

$$q_i^\pm = q(u_i^\pm) = q(u_i \pm \Delta u/2) \qquad (81)$$

The δ-function in Eq. (41) and (74) is approximated by a rectangular spike of thickness Δu and amplitude $1/\Delta u$. Separate the collision term in Eq. (80) into "diagonal" (i.e., containing $f_o(u_i) = f_i$) and "off-diagonal" elements (i.e. containing $f_o(u_i \pm u_\alpha)$) and use the detail balance relations (33) to define

$$D_i = \sum_\alpha \left[u_i N_\alpha Q_\alpha (u_i) + (u_i + u_\alpha) N_\alpha^* Q_\alpha (u_i + u_\alpha) \right] \qquad (82)$$

and

$$T_i = \sum_\alpha \Big[(u_i + u_\alpha) f_o(u_i + u_\alpha) N_\alpha Q_\alpha(u_i + u_\alpha) + u_i f_o(u_i - u_\alpha) N_\alpha^* Q_\alpha(u_i) \Big] \tag{83}$$

Eq. (80) can be rearranged to give

$$a_{i,i-1} f_{i-1} + a_{i,i} f_i + a_{i,i+1} f_{i+1} = b_i, \tag{84}$$

$i = 2, 3, \ldots, M$, to form a system of $(M-1)$ equations for M unknowns $(f_1, f_2, f_3, \ldots, f_M)$, with coefficients defined by

$$\begin{aligned}
a_{i,i-1} &= p_i^-/\Delta u - q_i^-/2 \\
a_{i,i+1} &= p_i^+/\Delta u + q_i^+/2 \\
a_{i,i} &= -(p_i^+ + p_i^-)/\Delta u + (q_i^+ - q_i^-)/2 \\
&\quad - \Delta u \Big[u_i^{1/2} (2e/m)^{-1/2} \dot{n}_e/n_e + D_i \Big] \qquad (85) \\
b_i &= -\Delta u \Big[T_i + (2e/m)^{-1/2} [S_i/n_e \\
&\qquad + \delta_{i,2} (\nu_i + S_o/n_e)/\Delta u] \Big],
\end{aligned}$$

for $i = 2, 3, \ldots, M$. Note that the diagonal terms have been placed on the LHS, and the off-diagonal terms on the RHS of Eq. (84). There is, obviously, considerable latitude in the definition of coefficients (e.g., Eq. (85)) for the reduction of the Boltzmann equation to the form (84). The essential criterion is that any such choice be suitable for numerical implementation by a convergent and computationally efficient algorithm for solution.

The set of (M - 1) equations (84) can be completed with an Mth equation in a variety of ways. The simplest approximation, which has been found to be quite satisfactory, is to take $f_1 = f_2$. After the iterative calculation of f converges, the magnitude is adjusted to satisfy the required normalization condition (48). Thus, Eq. (85) is supplemented by

$$a_{1,1} = b_1 = 0; \quad a_{1,0} = a_{1,2} = 0 \tag{86}$$

and the complete set of M equations in M unknowns can be written

$$\begin{aligned}
a_{1,1} f_1 & & & & & = b_1 \\
a_{2,1} f_1 + a_{2,2} f_2 + a_{2,3} f_3 & & & & & = b_2 \\
a_{3,2} f_2 + a_{3,3} f_3 + a_{3,4} f_4 & & & & & = b_3 \\
\vdots & & & & & \vdots \\
a_{M,M-1} f_{M-1} + a_{M,M} f_M & & & & & = b_M
\end{aligned} \tag{87}$$

in which form they resemble a linear tridiagonal system. It should be kept in mind, however, that they are neither linear or tridiagonal; the electron-electron scattering contribution makes p(u) and q(u) (and therefore, the coefficients $a_{i,i}$, $a_{i,i\pm 1}$) dependent upon $f_o(u)$, and the vector b_i contains off-diagonal elements $f_o(u_i \pm u_\alpha)$. Formally, the solution of the finite difference equations could be obtained (in the absence of electron-electron collisions, anyway) by direct matrix inversion, although this is not practical computationally or from the standpoint of computer storage requirements. Instead, the set of equations has been explicitly separated into the form of Eq. (87) in order to implement an iterative

technique which exploits the tridiagonal structure. Eq. (87) can be written in matrix form as

$$A(\vec{f})\vec{f} = \vec{b}(\vec{f}) \tag{88}$$

where

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & & & & \\ a_{2,1} & a_{2,2} & a_{2,3} & & & \\ & a_{3,2} & a_{3,3} & a_{3,4} & & \\ & & & \ddots & & \\ & & & & & a_{M-1,M} \\ & & & & a_{M,M-1} & a_{M,M} \end{bmatrix} \tag{89}$$

and $\vec{f} = (f_1, f_2, f_3, \ldots, f_M)^T$, $\vec{b} = (b_1, b_2, b_3, \ldots, b_M)^T$. The explicit dependence upon $\vec{f}$ of the matrix $A(\vec{f})$ and the vector $\vec{b}(\vec{f})$ has been expressed in Eq. (77), (78), (81), and (85). To solve the (nonlinear) equation (88), consider a sequence of vectors

$$\{\vec{f}^{\,i}\} = \vec{f}^{\,o}, \vec{f}^{\,1}, \ldots, \vec{f}^{\,n}, \vec{f}^{\,n+1}, \ldots \tag{90}$$

defined by the iterative equation

$$\begin{aligned} A(\vec{f}^{\,n})\vec{f}^{\,n+1} &= \vec{b}(\vec{f}^{\,n}) \\ \vec{f}^{\,n+1} &= A(\vec{f}^{\,n})^{-1}\vec{b}(\vec{f}^{\,n}), \end{aligned} \tag{91}$$

with the initial vector $\vec{f}^{\,o}$ chosen arbitrarily. If the sequence of vectors $\{\vec{f}^{\,i}\}$ defined by the recursion relation (91) converges, it must necessarily converge to the solution of Eq. (88), independent of the initial

guess chosen for $\vec{f}^{o}$. Since A is tridiagonal, it can be numerically inverted very rapidly by using elementary row manipulations downward (upward) to annihilate the lower (upper) diagonal, followed by back substitution upward (downward). Furthermore, the computer core requirements are substantially reduced, since only three diagonals (rather than a full M x M array) of elements need be stored and manipulated.

To implement the iterative technique, an initial guess for $\vec{f}^{o}$ is chosen and a sequence $\{\vec{f}^{i}\}$ of successively refined approximations is generated using Eq. (91). An acceptable approximation $\vec{f}^{n+1}$ to the solution of Eq. (88) is assumed to have been attained when the following convergence criterion is satisfied:

$$\mathrm{Max}_i \left| (f_i^{n+1} - f_i^n)/f_i^n \right| < \epsilon \tag{92}$$

The solution $\vec{f}$ to Eq. (88) is typically exponential, varying over several orders of magnitude in the range $(0, u_{max})$. Therefore, Eq. (92) has been weighted in such a way that the maximum <u>relative</u> (rather than absolute) change in all of the components f_i of the solution between two successive iterations must be less than ϵ for convergence to be declared. Eq. (92) is not rigorous, and probably requires mathematical assumptions about <u>uniform</u> convergence; however, it is physically reasonable and numerically convenient. (To illustrate the need for caution in applying Eq. (92), consider the sequence $\{S_n\}$ of partial sums, $S_n = 1 + (1/2) + (1/3) + \ldots + (1/n)$. For any fixed ϵ and for n sufficiently large, $(S_n - S_{n-1})/S_n = 1/nS_n < \epsilon$. Although the condition (92) predicts convergence at some point, the sequence $\{S_n\}$ is known to diverge.)

Note that all of the off-diagonal elements of the inelastic collision term

have been included in the vector $\vec{b}$, defined in Eq. (85). Terms involving an energy $(u_i \pm u_\alpha)$ are evaluated at the nearest mesh point, or are discarded if the energy lies outside of the range $[0, u_{max}]$ chosen for the calculations. (It is important, therefore, to choose a value for u_{max} that is suitably large to minimize computational inaccuracies that may result from such numerical "sinks". On the other hand, u_{max} cannot be chosen too large without sacrificing energy resolution.)

There are (at least in principle) an infinite number of ways in which Eq. (80) can be represented by a recursive sequence of equations such as (91). There is no a priori guarantee, in general, that an iterative procedure based upon an arbitrary definition of the coefficients for the recursive scheme of Eq. (91) will necessarily converge. In the course of development of the present algorithm, some variations in the definition of the coefficients $a_{i,j}$ and b_i were explored. For example, in an attempt to optimize performance, the definition (85) was modified by shifting a fractional part ξ of some of the diagonal terms in $a_{i,i}$ to the term b_i on the RHS of Eq. (84). It was found that, in some cases, the rapidity of convergence could be slightly enhanced by choosing $\xi > 0$, although problems were often incurred for large values of ξ ($\geqslant 0.4$) for which convergence was sometimes unsuccessful. It has been demonstrated by extensive numerical tests that the system of equations defined by Eq. (85)-(91) do converge (usually), and that they are quite efficient computationally. For the present analysis, therefore, the definition (85) has been adopted for the Boltzmann subroutine.

The coefficient $a_{i,i}$ defined by Eq. (85) contains the parameter $\dot{n}_e$, whose value is not known a priori. The first integral of the Boltzmann equation, Eq. (56), expresses $\dot{n}_e$ in terms of the secondary ionization, electron attachment and recombination, and external source creation rates. The frequencies ν_i and ν_a cannot be calculated without knowledge of the elec-

ledge of the distribution function $f_o(u)$. Therefore, a self-consistent iterative approach was taken to solve this problem.

An initial estimate (which may be zero) is assumed for $\dot{n}_e$, and the Boltzmann equation is solved recursively (as described above) until the convergence criterion of Eq. (92) is satisfied (with an initially coarse choice of ϵ, e.g., $\epsilon \sim .01$). The resulting distribution $f_o(u)$ is then used to calculate the secondary ionization, attachment, and recombination rates which can be used, along with the external creation rates, to obtain an improved estimate of $\dot{n}_e$ from Eq. (56). The procedure is repeated until the value for $\dot{n}_e$ converges to some acceptable accuracy. After convergence relative to the coarse parameter of accuracy is obtained, further refinement can be obtained by making the parameter ϵ smaller.

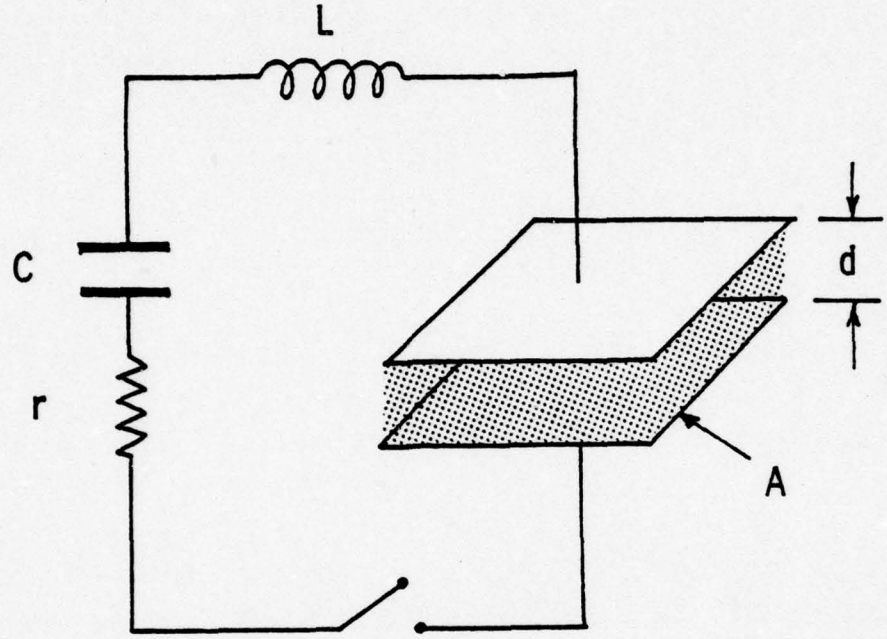
The implementation of these numerical algorithms is accomplished by a FORTRAN subroutine BOLTZ, to be described in more detail in Sec. 3.3 below. In addition, the subroutine is extensively documented with internal COMMENT cards (cf. listing in Vol. II). The present version of Program LASER uses the Boltzmann analysis only for the situation of an electric discharge, although in principle, the formulation should also be applicable to the case of direct e^--beam excitation only.

2.4 External Driving Circuit and Ionization Sources

A typical excitation scheme for high power electrical lasers employs a capacitive electric discharge, sustained by an external source of ionization such as a high energy electron beam. In some cases, the additional enhancement of electrical pump power provided by a discharge is not justified in terms of the additional complexity or problems that result, and direct excitation by e^--beam alone may be used. The present analysis includes external sources of ionization, as discussed in Sec. 2.3 for the electron kinetics, and couples the kinetic equations to the voltage and current equations for an external driving circuit.

The model for the external driving circuit is shown in Fig. 2.8. A plane parallel discharge of area A, with anode and cathode separated by a distance d, is driven by an external RLC circuit with a capacitor initially charged to a high voltage. This discharge is sustained by an external e^--beam whose temporal current density $J_b(t)$ can be specified as an arbitrary function of time. Initially, there is no voltage across the discharge because of the external circuit inductance. As the secondary electron density in the gas changes, the plasma conductivity (and hence the discharge impedance) will change. Thus, the plasma kinetics analysis is directly coupled to the circuit equations which define the instantaneous voltage $V_d(t)$ (and thus, $E(t)/N$) across the discharge. Although the present model for the external driving circuit is the simplest possible, it neverthless provides for the description of basic but important phenomena associated with pulsed excitation of the medium. If necessary, more sophisticated circuits (e.g., pulse-forming networks to better match impedance[5]) could be incorporated into the analysis.

EXTERNAL DRIVING CIRCUIT



Plasma conductivity: $\sigma = n_e(t) e \mu(t)$

Plasma impedance: $R_d(t) = d/A\sigma(t)$

$$L \frac{di}{dt} + (r + R_d(t))\, i + \frac{q}{C} = 0$$

Fig. 2.8: External RLC driving circuit excites gas in a plane-parallel discharge of area A, separation d.

The circuit equations will be formulated as first order differential equations for the charge q(t) and current i(t) in order to incorporate them on an equal basis with the molecular kinetic equations (4), the full set of which are integrated numerically using the Gear[6] technique. Thus,

$$dq/dt = i(t) \tag{93.1}$$

$$L\,di/dt = -q/C - (r + R_d(t))\,i \tag{93.2}$$

where L = inductance, r = external resistance, and C = capacitance. If the case L = 0 is desired, only one circuit equation is required:

$$dq/dt = q/(r + R_d(t))\,C \tag{94}$$

The discharge impedance $R_d(t)$ is a function of time, given by

$$R_d(t) = d/A\sigma(t), \tag{95}$$

where

$$\sigma(t) = n_e(t)\,e\,\mu(t) \tag{96}$$

is the plasma conductivity as a function of the instantaneous electron density $n_e(t)$ and the mobility $\mu(t)$. The voltage across the discharge,

$$V_d(t) = i(t)\,R_d(t) \tag{97}$$

determines the value of

$$E(t)/N = V_d(t)/dN \tag{98}$$

If Eq. (93.2) is multiplied by i(t), an expression for the conservation of energy (power) is obtained:

$$d/dt\,(Li^2/2) + i^2 r + (Ad)\sigma E^2 = -d/dt\,(q^2/2C). \qquad (99)$$

The physical interpretation of Eq. (99) is that the rate of change of stored inductive energy ($Li^2/2$), plus power dissipated in the external resistor ($i^2 r$) and deposited into the discharge, is equal to the rate of change of stored energy in the capacitor ($q^2/2C$). The discharge power density

$$\sigma E^2 = n_e(t)\, e\, \mu(t)\, E^2 \qquad (100)$$

has occurred previously in Eq. (67) for electrical power partitioning. In the following section, the overall power balance equation for the complete coupled system will be discussed.

2.5 Conservation of Energy

In the foregoing sections, 2.1 - 2.4, equations for power balance have been developed for each component of the coupled analysis. It is now appropriate to combine these results and to formulate a power balance relation for the complete system. The physical interpretation of the parameter $\Delta E(\alpha)$ for each reaction determines its physical significance in the power balance equation. To begin, therefore, some further discussion devoted to interpretation of the terms of Eq. (5) for specific types of kinetic reactions is required. This will provide the opportunity to describe the typical types of reactions permitted, and various conventions or restrictions on syntax.

Electron-Beam Collisions

It is beyond the scope of the present analysis to give a rigorous treatment of electron-beam energy deposition in a gas, although provisions have been made for the inclusion of high-energy electron collision processes in the molecular kinetic reaction scheme in terms of a simple rate constant formulation. Excitation and ionization of the molecular species X by collision with high-energy electrons $\vec{e}^-$,

$$X + \vec{e}^- \rightarrow X^* + \vec{e}^- + \Delta E \qquad (101.1)$$

$$X + \vec{e}^- \rightarrow X^+ + \vec{e}^- + e^-(u) + \Delta E \qquad (101.2)$$

are described in terms of cross sections σ^* and $\sigma^+(u)$, respectively. It is assumed that the medium is isotropically excited and "thin", so that the approximation of single scattering may be made. Adjustments for the effects of multiple scattering can be made in a qualitative way by multiplying the cross sections by an effective scale factor if some a priori knowledge of electron-beam deposition as a function of electron energy, gas mixture, and gas pressure is available. In terms of the e^--beam current density J_b (A/cm^2), the rates for reactions (101) are

$$-d[X]/dt = d[X^*]/dt = (J_b\sigma^*/e)[X] \qquad (102.1)$$

$$-d[X]/dt = d[X^+]/dt = (J_b\sigma^+/e)[X] \qquad (102.2)$$

where $\sigma^+ = \int du\sigma^+(u)$. The energies ΔE, as defined by Eq. (6), for the two reactions (101) are $\Delta E = -eu^*$ and $\Delta E = -eu^+$ respectively, where u^* and u^+ are excitation and ionization energies (eV). Thus, the contribution of e^--beam collisional excitation to the molecular power

balance Eq. (5) becomes

$$\sum_i (eu_i^*)\, d[X_i^*]/dt = J_b \sum_i u_i^* \sigma_i^* [X_i] \qquad (103.1)$$

$$\sum_i (eu_i^+)\, d[X_i^+]/dt = J_b \sum_i u_i^+ \sigma_i^+ [X_i] \qquad (103.2)$$

where the sums are over all species which are excited or ionized by the e^--beam. Strictly speaking, the reverse process for reaction (101.1) should also be included, although its contribution can usually be neglected in Eq. (103.1). When Eq. (67) for electron power balance is added to Eq. (5) for the molecular power balance, it is apparent that the contribution of the e^--beam will be given by

$$J_b\, dV/dx = J_b \sum_i \left[u_i^* \sigma_i^* + u_i^+ \sigma_i^+ + \int_0^\infty du\, u \sigma_i^+(u) \right] [X_i]$$

$$= J_b \sum_i \left[u_i^* \sigma_i^* + \left\{ u_i^+ + \langle U^+ \rangle \right\} \sigma_i^+ \right] [X_i], \qquad (104)$$

where dV/dx is an effective voltage drop for the beam, and the average energy $\langle U^+ \rangle$ deposited into the electron gas (defined originally in Eq. (69)) is given by the weighted average,

$$\langle U^+ \rangle \sum_i \sigma_i^+ [X_i] = \sum_i [X_i] \int_0^\infty du\, u\, \sigma_i^+(u). \qquad (105)$$

Cross section data for high-energy electron beam excitation has been given by Berger and Seltzer[23]. If multiple scattering effects are important for the physical problem to be analyzed, the Berger-Seltzer

cross sections can be appropriately adjusted by multiplying by some scale factor to produce an effectively larger deposition. The present analysis requires, as input rate constants, the total scattering cross sections σ_{i-}^{*} and σ_i^{+} for the e^--beam collision processes. In the case of excited state production, the information provided by σ_{i-}^{*} is sufficient. However, e^--beam ionization processes must be included in the source term (70) to the Boltzmann equation, and therefore, the detailed energy dependence of the cross section $\sigma_i^{+}(u)$ is required. For simplicity, it shall be assumed that the shape of the energy dependence is the same for all processes, so that the source term given by Eq. (70) can be written

$$S(u) = (J_b/e) \sum_i \sigma_i^{+} N_i \; s(u), \tag{106}$$

where s(u) is a normalized shape function satisfying

$$\int_0^\infty du \; s(u) = 1. \tag{107}$$

Thus, the average energy $\langle U^+ \rangle$ deposited as electron kinetic energy is

$$\begin{aligned} \langle U^+ \rangle &= \int_0^\infty du \, u \, s(u) \Big/ \int_0^\infty du \, s(u) \\ &= \int_0^\infty du \, u \, s(u) . \end{aligned} \tag{108}$$

The total rate of creation of secondary electrons by e^--beam ionization (cm^{-3}/s) is thus

$$S_b = \int_0^\infty du\, S(u) = (J_b/e) \sum_i \sigma_i^+ N_i \int_0^\infty du\, s(u) = (J_b/e) \sum_i \sigma_i^+ N_i, \quad (109)$$

as given by Eq. (68), and the energy deposition rate (i.e., power density, W/cm^3) is

$$\int_0^\infty du\,(eu)\, S(u) = e S_o \int_0^\infty du\, u\, s(u) = e \langle U^+ \rangle S_b, \quad (110)$$

where $e = 1.602 \times 10^{-19}$ J/eV. For convenience, the normalized shape function s(u) is defined (by input) to be a square wave,

$$s(u) = \begin{cases} 0, & u < u_a, \\ 1/(u_b - u_a), & u_a \leq u \leq u_b, \\ 0, & u > u_b, \end{cases} \quad (111)$$

and thus,

$$\langle U^+ \rangle = (u_a + u_b)/2. \quad (112)$$

Because the present approach to e^--beam deposition is phenomenological with no <u>a priori</u> knowledge of energy dependence, the simplified assumptions for s(u) must suffice. Furthermore, it should also be noted that the present formulation of e^--beam excitation and ionization collisions does not provide an explicit mechanism for heating the gas by direct deposition into molecular kinetic energy. The phenomenological description of e^--beam deposition should be sufficiently flexible to be applicable to typical situations of interest. Where the approximations are inadequate, the analysis must necessarily be extended as required.

Secondary Electron Creation

In addition to e^--beam ionization, there are a variety of kinetic mechanisms which involve the creation of secondary electrons. It is appropriate to make some comments here with regard to the manner in which such processes are to be included in the Boltzmann analysis, and to discuss the resulting consequences for the power balance equation.

In general, any kinetic reaction which involves the creation of secondary electrons must be accounted for in the source term $S_{ext}(u)$ for the Boltzmann equation. The contribution of e^--beam ionization to $S(u)$ is given by Eq. (106). Other electron creation processes could include, for example,

Photoionization: $A + I(\nu) \rightarrow A^+ + e^-$

Photodetachment: $A^- + I(\nu) \rightarrow A + e^-$

Penning Ionization: $A^* + B \rightarrow A^+ + B + e^-$

Since there is no a priori knowledge of the kinetic energy distribution of the created secondary electrons, it is convenient to assume that they are all created at zero energy and that the remaining energy ΔE is converted to molecular kinetic energy. (This is analogous to the treatment of electrons created by secondary ionization.) The contribution from such processes to the source term is proportional to a δ-function:

$$S_{ext}(u) = (J_b/e) \sum_i \sigma_i^+ N_i \, s(u) + \delta(u) \Big[I\sigma_{ph}[A]/h\nu + I\sigma_{pd}[A^-]/h\nu + k_{PI}[A^*][B] + \ldots \Big] \qquad (113)$$

The δ-function term makes no contribution to electrical power balance.

Secondary Electron Collisions

For a binary electron-molecule collision,

$$X + e^- \rightarrow X^* + e^- + \Delta E$$

the energy ΔE is given by $\Delta E = -eu^*$, where u^* is the inelastic energy loss (eV) for the process. Thus, the contribution of secondary electron collisions to the right hand side of the molecular power balance Eq. (5) is

$$-\sum_{\alpha} R(\alpha)\Delta E(\alpha) = n_e \sum_{\alpha} (eu_\alpha)\left[N_\alpha \langle v Q_\alpha \rangle - N_\alpha^* \langle v Q_{-\alpha} \rangle\right] \qquad (114)$$

Note that the sum on the right hand side of Eq. (114) is not restricted to exclude attachment (or recombination) processes, as was the case in Eq. (67) for electrical power balance. For attachment and recombination, denoted by "a", the difference

$$n_e N_a e(2e/m)^{1/2} \int_0^\infty du\, u^2 f_o(u) Q_a(u) - n_e N_a (eu_a)\langle v Q_a \rangle$$

$$= n_e N_a e(2e/m)^{1/2} \int_0^\infty du\, u(u - u_a) f_o(u) Q_a(u) \qquad (115)$$

can be interpreted as (a contribution to) the kinetic heating of the molecular gas mixture. For example, in a "two-body" recombination process such as

$$X^+ + e^- \rightarrow X \qquad (116)$$

the ionization energy u^+ and the electron kinetic energy are converted to kinetic energy of X and to recombination radiation energy $u_r = h\nu_r$ of a photon (which has been tacitly suppressed in (116)). Since u_a (= $-\Delta E$) = $-u^+$ for reaction (116), the resulting power density is

$$P = en_e[X^+](2e/m)^{1/2}\int_0^\infty du\, u\left[(u + u^+ - u_r) + u_r\right] f_o(u)\, Q_r(u), \quad (117)$$

where $Q_r(u)$ is the recombination cross section. The first term represents conversion of energy to molecular kinetic energy, and the second to radiation. In the subsequent discussion, we shall neglect the distinction, and simply interpret Eq. (117) as molecular kinetic heating.

Radiative Processes

Both spontaneous as well as stimulated emission and absorption processes can be included in the present analysis. In addition to stimulated processes involving the laser transition, absorption of laser radiation by other species may also occur. There are certain distinctions and conventions that must be observed in the present analysis, and the corresponding interpretations for the power balance equation will be discussed.

First of all, spontaneous emission photons (except for those which build up the laser field) are neglected as independent species in the reaction syntax, specified by

$$X^* \rightarrow X. \quad (118)$$

The contribution of this reaction to the right hand side of Eq. (5) is just

$$-R\Delta E = -eu^*[X^*]/\tau_{sp} \quad (119)$$

where $\Delta E = eu^*$ is the energy defined by Eq. (6), and τ_{sp} is the spontaneous radiative lifetime. For all of the spontaneous emission processes from excited states, the terms of the form (119) can be interpreted as fluorescence loss. The syntax of Eq. (118), which explicitly omits reference to the radiated photon, is recognized by the computer analysis to represent spontaneous emission.

For the photon field of the laser, however, the syntax for defining spontaneous radiation is

$$X^* \rightarrow X + h\nu, \tag{120}$$

where the emitted photon must be <u>explicitly</u> indicated. The reason for this is that the laser field is defined in terms of the intracavity photon number density, and laser photons are treated as species on an equal basis with electrons, ions, molecules, and all of the other "particle" species which occur in the kinetic reaction scheme. To insure a parallel treatment, some further observations and definitions must be made.

First of all, since the volume of the active gain medium is less than the cavity volume by a factor (L_g/L_c), it is appropriate to define

$$N_{ph} = (L_c/L_g)\, n_{ph} \tag{121}$$

as an effective photon number density in the gain medium (as if the radiation were considered to be confined to the gain volume). This is logical, since the power balance Eq. (5) is formulated in terms of the <u>power density</u> in the gain medium, and all of the other species are described by their population densities in the gain medium. In terms of the photon

density N_{ph}, the intracavity intensity is

$$I = (L_g/L_c)\, ch\nu\, N_{ph}, \tag{122}$$

and the radiation Eq. (13) becomes

$$dN_{ph}/dt = (\Omega/4\pi)\, N^*/\tau + (L_g/L_c)\, c\left[\alpha(t) - \alpha_{th}\right] N_{ph}. \tag{123}$$

$\alpha(t)$, the instantaneous net gain coefficient, was defined in Eq. (10), and α_{th} is the threshold loss coefficient, given by

$$\alpha_{th} = \left[\gamma + (1/2)\ln(1/R)\right]/L_g, \tag{124}$$

where γ is the intracavity loss per pass (i.e. from optical elements), and R is the output coupling reflectivity. The total contribution from output coupling and the radiative processes of Eq. (7), (8), and (120) to the power balance equation (5) is

$$\sum_A E_A\, d[A]/dt + \sum_{A^*} E_{A^*}\, d[A^*]/dt + h\nu\, dN_{ph}/dt$$

$$+ E_{X^*}\, d[X^*]/dt + E_X\, d[X]/dt = -\left[1 - (\Omega/4\pi)\right][X^*]\, h\nu/\tau$$

$$- (I/h\nu) \sum_A \sigma_A [A] (E_A - E_{A^*} + h\nu) - I\alpha_{th} \tag{125}$$

The interpretation of the terms of Eq. (125) is straightforward. On the left hand side, there is the rate of change of stored energy density. The first term on the right hand side represents the net fluorescence power loss from reaction (120), and is consistent with the assumption that a fractional part ($\Omega/4\pi$) of the spontaneous emission photons are not lost, but remain in the cavity to build up the optical field. Reference to Eq. (8) shows that the energy difference ($E_A + h\nu - E_{A^*}$) corresponds to the net energy converted to kinetic energy of the species A^*. Thus, the second term on the right hand side of Eq. (125) can be interpreted as a kinetic heating power density. The third term corresponds to optical loss, due to absorption by intracavity optical elements (γ), and output coupling (R).

Kinetic Heating

With the exceptions noted above, the energy change ΔE defined by Eq. (6) for the reaction (1) is the net energy converted to molecular kinetic energy, and thus, the physical significance of the term

$$\sum_{\beta} R(\beta)\, \Delta E(\beta)$$

on the right hand side of Eq. (5) is that it represents power density into kinetic heating of the molecular gas. The exceptions which occurred were the result of the tacit suppression of some species involved (e.g., the emitted photon in spontaneous radiation) or of the kinetic energy dependence of some of the interacting species (e.g., secondary and high-energy e^--beam electrons). In the case of secondary electrons, for which an integration over a continuum of energies is required, the contribution to the power balance must be derived from the Boltzmann equation.

Total Power Balance for the Coupled System

As a result of the foregoing discussion, which should clarify the physical significance of the terms of Eq. (5), it is now possible to construct the equation for conservation of power density for the coupled system of electrons, molecules, radiation, and external driving circuit. If Eq. (5) is added to the expression given by Eq. (67) for $e\bar{u}\,dn_e/dt$, and the terms are rearranged, the following result is obtained:

$$\sum_i E_i\, d[X_i]/dt + h\nu\, dN_{ph}/dt + e\bar{u}\, dn_e/dt + \sum_A h\nu_A [A^*]/\tau_A$$

$$+ \left[1 - (\Omega/4\pi)\right] h\nu [X^*]/\tau + I\alpha_{th} + \sum_\beta{}' R(\beta)\Delta E(\beta)$$

$$+ en_e \sum_{a,r} N_a \left[(2e/m)^{1/2} \int_0^\infty du\, u^2 f_o(u) Q_a(u) - u_a \langle v Q_a(u) \rangle \right]$$

$$+ en_e (2e/m)^{1/2} \int_0^\infty du\, u^2 \langle (2m/M) N Q_m \rangle \left[f_o + (kT/e)\, df_o/du \right]$$

$$= \sigma E^2 + J_b \sum_k \left[u_k^* \sigma_k^* + [u_k^+ + \langle U^+ \rangle] \sigma_k^+ \right] [X_k]$$

$$= \sigma E^2 + J_b\, dV/dx. \qquad (126)$$

The first three terms on the left correspond to the rate of change of the energy density stored in the molecules, radiation field, and electrons. The sum over i excludes electrons, but photons (which have been shown explicitly in the second term) could be included in that sum by defining

$E_i = h\nu$ for that "species". The fourth and fifth terms represent spontaneous fluorescence loss, while the sixth is the optical power loss by intracavity absorption and output coupling. The remaining terms on the left hand side have the significance of kinetic heating of the molecular gas. The sum over β in the seventh term includes all processes except spontaneous emission, secondary electron collisions, and high-energy e^--beam collisions. All resonant energy transfer processes (i.e. for which $\Delta E = 0$) contribute nothing to the sum over β, nor does the stimulated emission reaction, since $\Delta E = E_{X^*} - E_X - h\nu = 0$. The eighth term consists of the net contribution to molecular heating from recombination and attachment processes, assuming that recombination radiation is neglected. The last term on the left hand side is the power density into elastic heating from electron-molecule momentum transfer collisions.

On the right hand side, there is the input electric discharge power density σE^2 and the beam deposition $J_b\, dV/dx$, where the effective e^--beam voltage drop dV/dx was defined in Eq. (104). The discharge power density σE^2 can be expressed in terms of the parameters of the external driving circuit by Eq. (99).

In its present formulation, the coupled analysis assumes that the molecular temperature of the gas remains constant. This restriction could easily be removed, if necessary, by an additional equation

$$C_v\, dT_{mol}/dt = \sum_{\beta} R(\beta)\Delta E(\beta) + \text{misc. heating terms} \qquad (127)$$

where C_v is the specific heat of the gas at constant volume ($J/cm^3\,K$), and the right hand side is the total power density into kinetic heating.

The numerical solution of the coupled system of molecular and electron kinetic equations proceeds as follows. The total pulse duration is divided into a specified number (e.g., 200) of (equal) subintervals defined by a time grid $[0, t_1, t_2, \ldots, t_k, \ldots]$. At each of the discrete points t_k in time, the Boltzmann equation is solved (as a function of the instantaneous values $E(t_k)/N$ and the excited state population densities $N_\alpha(t_k)$) to update the electron excitation rates $\langle v Q_\alpha \rangle$ and plasma parameters, which are then assumed to remain constant over the following subinterval $[t_k, t_{k+1}]$ of time. The molecular kinetic (and circuit) equations are integrated over this subinterval, and in practice, the integration step size will usually be much smaller than the coarse time intervals $[t_k, t_{k+1}]$ over which the electron kinetics calculations are performed. The Gear[6] technique automatically adjusts the step size to maintain accuracy and stability.

The assumption that the electron energy distribution function $f_o(u)$ is constant over these discrete subintervals will result in a power balance discrepancy in the calculations. Assume that $f_o^k(u)$, $\langle v Q_\alpha \rangle_k$, μ_k, $\bar{u}_k$, ... represent the electron distribution, excitation rates, mobility, average energy, etc. obtained from solution of the Boltzmann equation at some discrete point $t = t_k$. If Eq. (67) were to be numerically evaluated at a later time t by the approximations that $f_o(u) = f_o^k(u)$, $\langle v Q_\alpha \rangle = \langle v Q_\alpha \rangle_k$, $\bar{u} = \bar{u}_k$, $\mu = \mu_k$, ... the right hand side would contain an additional term δP representing a power discrepancy:

$$\delta P(t_k, t) = e n_e(t) \mu_k E(t)^2 + e \langle U^+ \rangle S_b(t) - e \bar{u}_k \, dn_e(t)/dt$$

$$- n_e(t)\, e (2e/m)^{1/2} \int_0^\infty du\, u^2 \langle (2m/M) N Q_m \rangle \left[f_o^k(u) + (kT/e)\, df_o^k(u)/du \right]$$

(continued)

$$- n_e(t) \sum_{\alpha} (eu_{\alpha}) \left[N_{\alpha}(t) \langle v Q_{\alpha} \rangle_k - N^*_{\alpha}(t) \langle v Q_{-\alpha} \rangle_k \right]$$

$$- n_e(t)\, e(2e/m)^{1/2} \sum_a N_a(t) \int_o^{\infty} du\, u^2\, f_o^k(u)\, Q_a(u) . \tag{128}$$

Since $f_o^k(u)$ and the corresponding plasma parameters and excitation rates are recalculated at the point t_{k+1}, the longest period of time over which the approximation $f_o(u) = f_o^k(u)$ is sustained is the length of the discrete interval, $\Delta t = t_{k+1} - t_k$. Therefore, a useful measure of the accuracy of the calculation (at least insofar as it is affected by errors resulting from the discrete time partition) should be

$$\xi(t_k, t) = P(t_k, t)/P_{tot}(t), \tag{129}$$

where

$$P_{tot}(t) = e n_e(t)\, \mu(t)\, E(t)^2 + J_b(t)\, dV/dx \tag{130}$$

is the total electrical input power density. If Eq. (128) is evaluated at the time $t = t_k$, a measure of power balance inaccuracy resulting from the numerical solution of the Boltzmann equation is obtained. (Since it is only the contribution $e\langle U^+ \rangle S_b$ to $J_b dV/dx$ that occurs in the electron kinetics analysis, the fractional power discrepancy reported from the Boltzmann calculations is normally defined in terms of total electrical excitation power density,

$$P_e = e n_e \mu E^2 + e \langle U^+ \rangle S_b . \tag{131}$$

The present formulation of the coupled system of equations makes the

tacit assumption that the charge $q(t)$, current $i(t)$, and all of the population densities $N_\alpha(t)$ are continuous from $t_k^- = t_k - 0$ to $t_k^+ = t_k + 0$:

$$
\begin{aligned}
i(t_k^-) &= i(t_k^+), \\
q(t_k^-) &= q(t_k^+), \\
N_\alpha(t_k^-) &= N_\alpha(t_k^+),
\end{aligned}
\tag{133}
$$

and thus, these quantities can always be defined unambiguously as functions of the time t_k. However, all of the electron parameters and excitation rates are discontinuous from t_k^- to t_k^+, since they are updated at $t = t_k$ by a new solution of the Boltzmann equation. Furthermore, the derivatives $di(t)/dt$, $dn_e(t)/dt$, and $dN_\alpha(t)/dt$ for all species α which are involved in secondary electron collision processes will also be discontinuous. At $t = t_k^-$, just prior to the Boltzmann update, the electric field is obtained from

$$
E_k = E(t_k^-) = i(t_k)R_d(t_k^-)/d = i(t_k)/[Aen_e(t_k)\mu(t_k^-)], \tag{134}
$$

and the fractional power discrepancy $\xi(t_k, t_k)$ defined by Eq. (128) and (131) is based upon the assumption that E_k is the electric field. However, the plasma conductivity $\sigma = en_e\mu$ (and thus, the discharge impedance $R_d = d/A\sigma$) are discontinuous from t_k^- to t_k^+, and therefore, the electric field at $t = t_k^+$ is

$$
E_k^+ = E(t_k^+) = i(t_k)/[Aen_e(t_k)\mu(t_k^+)] = (\mu_k^-/\mu_k^+)E_k. \tag{135}
$$

Thus, in addition to the power discrepancy $\delta P(t_k, t_k)$ inherent in the numerical solution of the Boltzmann equation, there will also be an imme-

diate discrepancy associated with the discontinuity in the electric field:

$$\delta P(t_k, t_k^+) = \delta P(t_k, t_k) + en_e(t_k)\mu(t_k^+)\left[(E_k^+)^2 - E_k^2\right]$$

$$= \delta P(t_k, t_k) + en_e(t_k)\mu_k^+ E_k^2\left[(\mu_k^-/\mu_k^+)^2 - 1\right], \qquad (136)$$

where $\mu_k^+ = \mu(t_k^+)$. There are three fractional power discrepancies which are a useful measure of the accuracy of the calculations. The first is the inherent power accuracy of the numerical solution of the Boltzmann equation,

$$\xi_k^o = \delta P(t_k, t_k)/P_e, \qquad (137)$$

and it is provided as part of the output summarizing the results of the electron kinetics analysis. The second is

$$\xi_k^- = \xi(t_{k-1}, t_k^-) = \delta P(t_{k-1}, t_k^-)/P_{tot} \qquad (138)$$

which represents the cumulative error which has developed over the entire preceding subinterval of time. The third is

$$\xi_k^+ = \xi(t_k, t_k^+) = \delta P(t_k, t_k^+)/P_{tot} \qquad (139)$$

which represents the fractional additional error resulting from discontinuity in the electric field before and after the Boltzmann update. If ξ_k^+ or ξ_k^- are too large, the length $\Delta t = t_{k+1} - t_k$ of the subintervals should be reduced.

3.0 COMPUTER PROGRAM DESCRIPTION

The generalized laser kinetics code has been written in FORTRAN IV, and was developed for use with the Extended FORTRAN Compiler of the CDC 6000 and CYBER Series of computers (SCOPE 3.4). If it is necessary to execute this program on a different computer system, some modifications of nonstandard syntax or conventions may be required. In addition, extensive usage of ENCODE and DECODE statements (for output formatting) makes the explicit assumption that the basic "word" size is 60-bit, 10-BCD character display. Modification of such statements will be necessary if the program is to be adapted to a computer with a different word size.

The program structure, flow diagrams, description of subroutines, control card commands and requests, external file usage, input card format and default conditions, available output options, and illustrative input and output from a sample case will all be described. The complete FORTRAN program listing is given in Vol. II of the present report. In addition, Vol. II also contains a listing for an electron kinetics analysis program, which makes use of the same subroutines.

3.1 Program Structure and Flow Diagram

The program structure has been designed with the objective of providing maximum input and output flexibility, while reducing mechanical programming tasks for the user to a minimum. A given kinetic reaction scheme is specified by input (with a completely free and flexible syntax) as a sequence of symbolic reactions containing an arbitrary number of processes and interacting species. These reactions are translated into computer-coded FORTRAN equations to generate molecular kinetics subroutines, which are then combined with the master

executive program LASER and (seventeen) other subroutines to form a completely self-contained source program for the coupled analysis based upon the specified reaction scheme (cf. Fig. 2.3).

Fig. 3.1 presents a more detailed flow diagram of the main program LASER. Initially, there may or may not be a synthesized program available, and the control cards and data input deck structure must be compatible so that LASER can execute either situation. Initially, the program makes an attempt to read "TITLE" on an attached file TAPE4, which would normally contain the "name" and miscellaneous rate constant data associated with a synthesized reaction scheme of a previous run. If an EOF is encountered on the attempt to read file TAPE4, the program assumes that user intends to generate subroutines and a data file for a new reaction scheme, to be specified by input DATA BLOCK 1. In that case, the input of DATA BLOCK 1 is processed by Subroutine SYNTH, which translates the reaction structure into three subroutines (DNDT, JACOB, and LEVELS) which consist of 80-BCD character records on file MTAPE (= 3). Furthermore, as the reaction scheme of DATA BLOCK 1 is processed, miscellaneous data is written onto file TAPE4. Diagnostics are generated for a variety of error conditions which may be encountered. Although synthesis proceeds by ignoring unacceptable syntax or other errors, protection against subsequent execution of a faulty reaction scheme can be obtained by declaring such conditions to be fatal. After files TAPE4 and TAPE3 are constructed, EXIT occurs, the synthesized subroutines are compiled and combined with the other subroutines, and LASER is again executed. This time, TAPE4 contains reaction scheme data, and the attempt to read "TITLE," the "name" of the synthesized program, is successful. Control transfers to Read DATA BLOCK 2, which contains input electron cross section data.

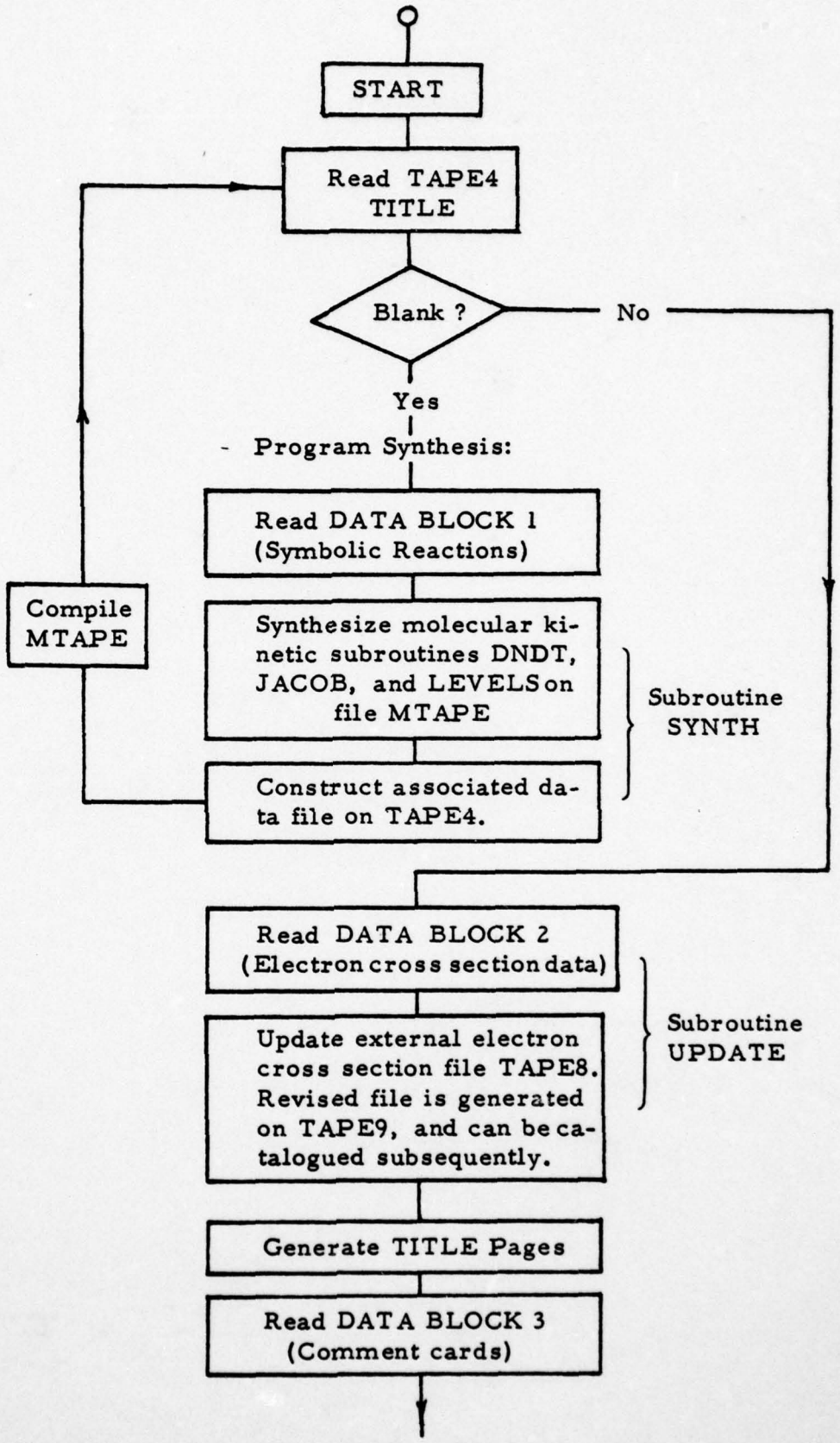


Fig. 3.1: Flow diagram of LASER Synthesis Code.

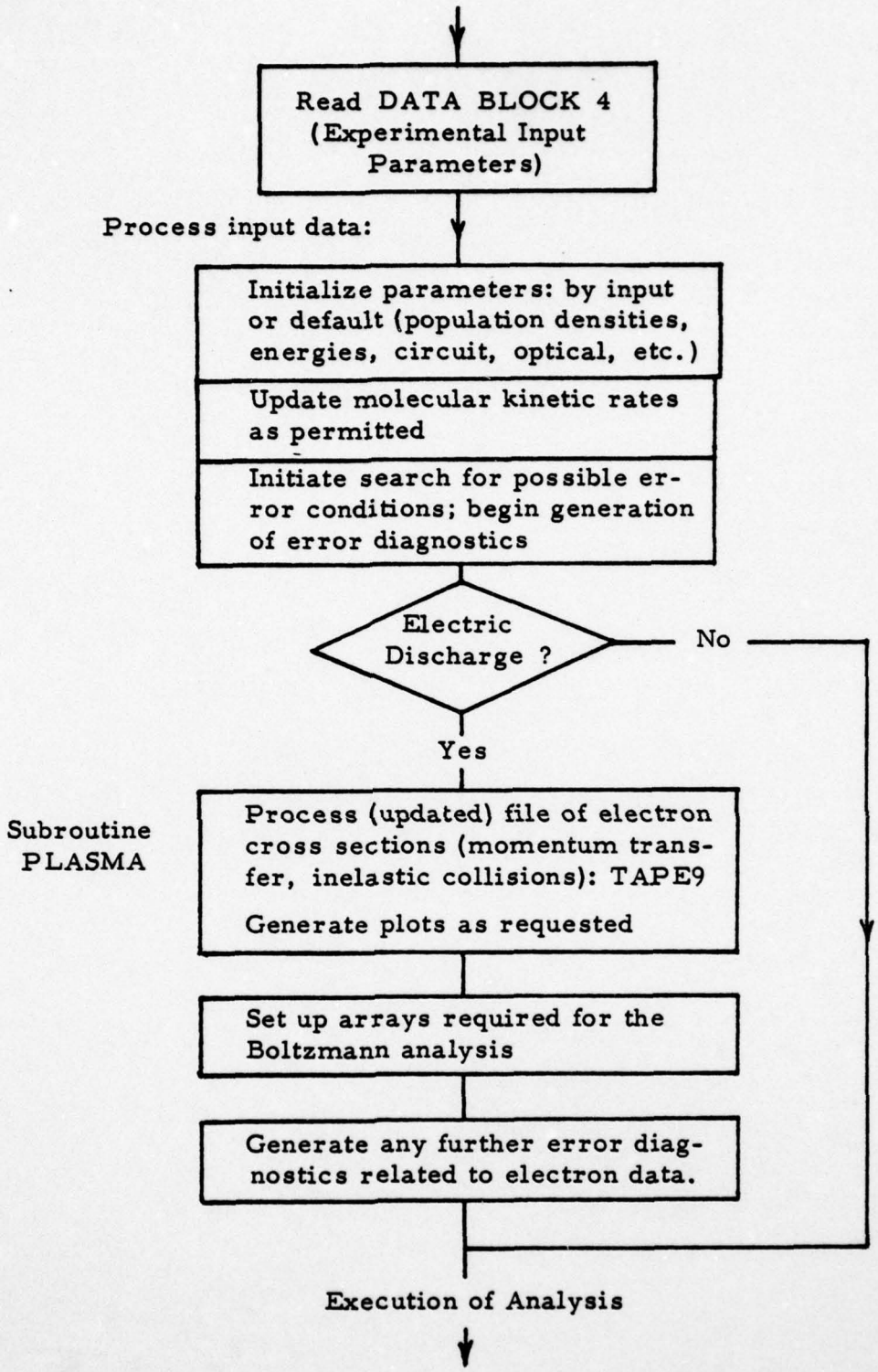


Fig. 3.1: Flow Diagram of LASER Synthesis Code (cont'd).

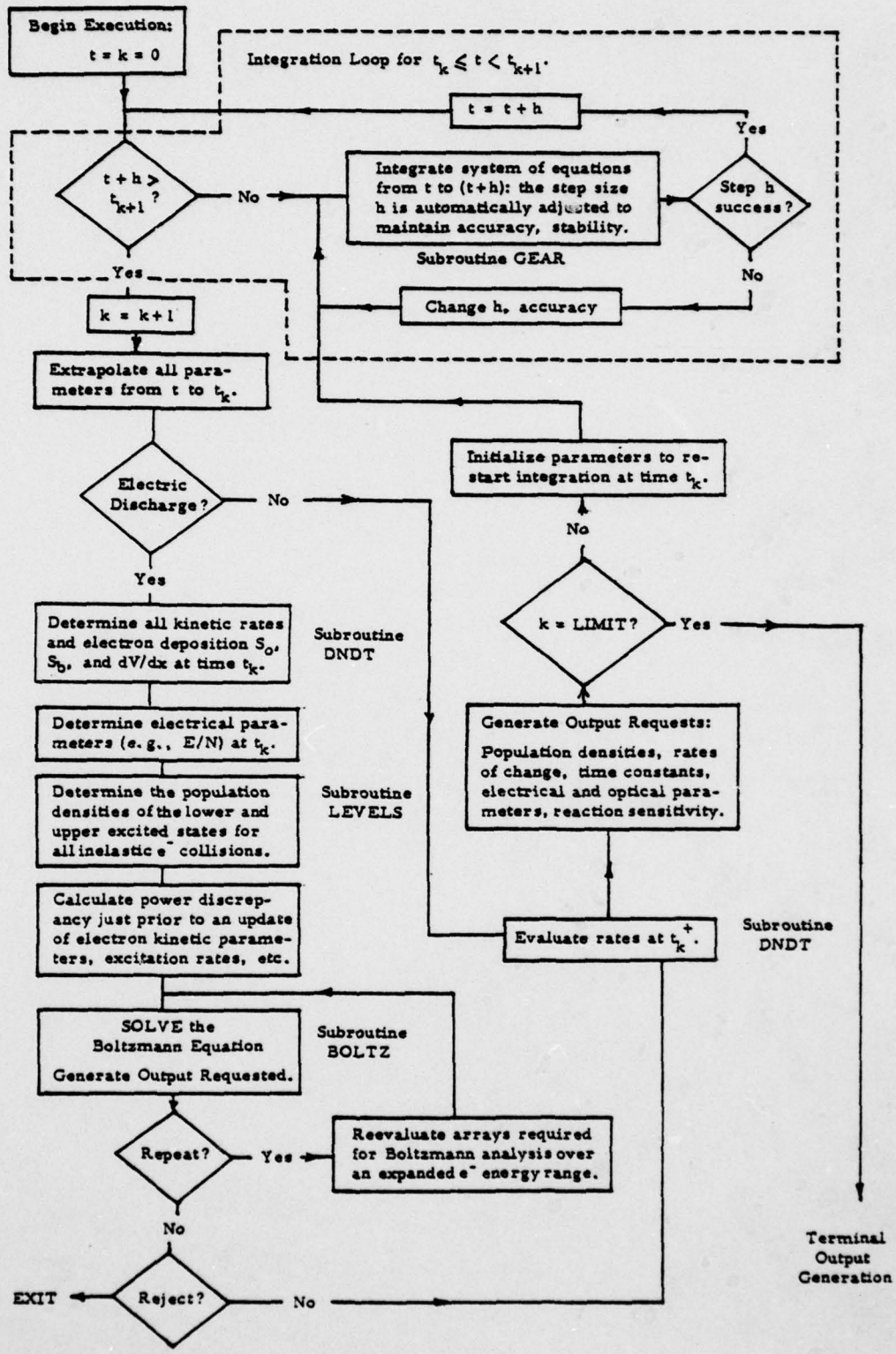


Fig. 3.1: Flow Diagram of LASER Synthesis Code (cont'd).

Electron cross section card data is entered by DATA BLOCK 2 to update a main electron cross section library, which is provided on file TAPE8. The updated library, which is generated on TAPE9, may be catalogued for future use if desired. DATA BLOCK 2 may be completely empty, or it may contain extensive data; indeed, the initial library itself can be constructed by "updating" an empty file on TAPE8 and cataloging the resulting TAPE9. During subroutine synthesis and reaction processing, a search is made (for each secondary electron collision encountered) to determine whether the appropriate cross section data is available in the external library. If it is not, a warning diagnostic is generated. The only cross section data available at the time of program synthesis is the original data on TAPE8. An omission error, which would most likely be declared fatal initially, could always be removed by an electron file update on a subsequent run.

DATA BLOCK 3 contains comment cards which are reproduced in the output. DATA BLOCK 4 contains the experimental input parameters for execution of the analysis. The input data is processed and all of the run parameters are initialized (explicitly or by default). The molecular kinetic rate constants are updated, as permitted.

At the time of subroutine synthesis, reactions are defined by their forward and reverse rate constants. If a rate constant (e.g., for the reverse reaction) was zero, no translation of that term occurs and no subsequent modification of that rate is accessible to input. For secondary electron collisions, however, the appearance of a zero rate constant automatically produces a default to the Boltzmann analysis. If a nonzero rate constant was initially provided (at the time of synthesis) for a secondary electron process, no coupling of that process to the Boltzmann analysis occurs. No subsequent modification of a rate

constant which defaults to the Boltzmann analysis is permitted. An exception occurs for the situation of no electric discharge, in which case, input modification of a secondary electron rate is accepted. A detail balance relation is enforced for binary collisions, with the reverse rate defined in terms of the product of the forward rate and an exponential factor. Therefore, reverse rate constants for such processes cannot be modified either. An illegal attempt to modify rates inaccessible to input in DATA BLOCK 4 is detected (and ignored) and an error diagnostic is generated.

The analysis is executed by subdividing the total pulse time TPULSE into NCYCLE (equal) subintervals of time Δt = TPULSE/NCYCLE, defining a partition of discrete times $t_k = k\Delta t$ ($k = 0, 1, 2, \ldots,$ LIMIT). At each of these discrete times, the Boltzmann equation is solved to update the electrical parameters and electron excitation rates, and a variety of output option requests can be specified. Normally, TPULSE is the total pulse interval, and LIMIT = NCYCLE; however, the combination of parameters TPULSE, NCYCLE, and LIMIT provides more flexibility for the joint specification of total integration time and the frequency of electron kinetic updates and output generation. Over the subinterval $t_k \leq t < t_{k+1}$, the coupled molecular and circuit equations are integrated using a multistep Gear technique[6], shown in the dashed box in Fig. 3.1. If the current integration step size is h and the time is t, the program tests whether an additional integration to time (t + h) would exceed the next cycle time t_{k+1}; if so, program resets the cycle count to (k + 1) and extrapolates all parameters from time t to time t_{k+1} by the use of an array (provided by Subroutine GEAR) which contains population densities and their derivatives (to various orders). If (t + h) would not have exceeded the next discrete cycle point, the GEAR subroutine continues the integration across the

subinterval. Subroutine GEAR automatically adjusts the step size h to maintain accuracy and stability.

If the amount of time consumed by the Boltzmann updates and output generation at a cycle time t_k were negligible, the total CP time for execution of the complete analysis should be independent of NCYCLE, since the integration would only be interrupted by brief pauses at k = 0, 1, 2, . . . In actual fact, these additional tasks performed at the cycle times t_k do consume only a small fraction of the total computation time for integration from t_k to t_{k+1}. However, it has been observed (from actual runs of the program) that the total CP execution time seems to increase proportionately with (rather than be relatively independent of) NCYCLE. At the discrete time t_k, after the electron kinetic calculations and output generation, the GEAR integration must be restarted (with JSTART = 0). For the case of an electric discharge, some of the kinetic rate constants (i. e., those for the secondary electron collisions) change from $t = t_k^-$ to $t = t_k^+$, and it is possible that the restart process consumes an excessive time before the step size can be finally increased to its most economical size. So long as the integration loop in the dashed box is not disturbed, execution is efficient and an economically large step size is attained and maintained. However, an exit and subsequent return to the integration loop with a restart seems to cause the problem. (The problem does not seem to arise for calculations involving no electric discharge.) There has not been adequate opportunity to explore conclusively the origins of this difficulty, or to optimize the execution time. However, it is quite likely that significant improvement in execution efficiency should be possible with only minimal modifications in the integration technique. In any case, for the present version of the program, it is advantageous to use a relatively small (e.g., 50, 100) value of NCYCLE.

After k = LIMIT is attained, execution terminates and control is transfered to final output generation. This includes miscellaneous tables and plots of electrical and optical quantities, molecular population densities, etc. as a function of time.

The listing of the program, which appears in Vol. II, contains extensive COMMENT card documentation of additional information which is too detailed to be described here. As most of the FORTRAN variable names have been chosen to be reasonably descriptive of the physical quantities they represent, it is believed that the logical and computational structure of the program should be relatively straightforward when supplemented with Fig. 3.1 and the present discussion.

The program has been written in such a way that dimension storage can be changed relatively easily. Arrays are communicated to subroutines by variable dimension calls and thus, it is sufficient to define a set of DIMENSION declarators which can be easily modified. The DIMENSION statement changes required are described by COMMENT cards in the listing. The only other precaution that must be observed is that labelled COMMON blocks shared with subroutines synthesized in previous runs must be consistent.

External file usage (TAPE2, TAPE3, ..., TAPE10) is as follows: TAPE2 is a scratch file used in subroutine synthesis and analysis of reaction sensitivity. TAPE3 and TAPE7 are used for writing the FORTRAN translation of the symbolic reaction scheme; they are subsequently combined on TAPE3, which provides a source file of 80-BCD character records of the statements of the synthesized subroutines JACOB, DNDT, and LEVELS which can be compiled. TAPE4 is a file provided for writing miscellaneous reaction data associated

with a specified kinetic scheme. TAPE4 contains data which is an essential supplement to the synthetically generated program, and it must be catalogued and saved if future execution is intended. TAPE3 (which consists of 80-BCD character records which are the FORTRAN statements of the synthesized subroutines) can be used as the input source for creation of an UPDATE program library, which can be catalogued and saved if any future specialized modifications (beyond the scope of the synthesis capability of LASER) are anticipated. Normally, it would be sufficient to catalog and save the binary compilation of subroutines DNDT, JACOB, and LEVELS for future execution. Thus, even for specialized situations for which LASER may not be totally adequate for synthesizing the exact structure desired for the rate subroutines, it is always possible to revise the source program generated by means of subsequent update procedures.

TAPE8 is used for at attached file of electron cross section data. The electron cross section library can be updated by DATA BLOCK 2 card input to form a revised file on TAPE9, which can be catalogued and saved for future use as desired. TAPE10 is the card input file; a processing subroutine EDITOR reads card input data to an EOF on unit 10 and generates an output playback of the card images. It also copies the card images onto TAPE5, creating an effective card input file on unit 5. Each time a new data block (terminated by an EOF card) is encountered, playback of card images and creation of an effective input file TAPE5 occurs. TAPE6 is used for OUTPUT.

In the following sections, some of the important subroutines will be discussed in more detail. The card format for the input data decks will be described, and the instructions for usage illustrated with sample control cards.

3.2 Input Data Description

Input to the code consists of card and/or tape (disc) data files. As the flow diagram of Fig. 3.1 indicates, there are four main blocks (DATA BLOCK 1, 2, 3, and 4) of card input; in addition, an external file (TAPE8) containing an electron cross section library may also be attached. In this section, a description of the card input sequences, with format specifications and physical units assumed, will be given. The external cross section file (attached on TAPE8) is originally created with card input from DATA BLOCK 2.

In order to provide maximum flexibility for data input with a minimum number of format restrictions, NAMELIST entry is frequently used. Various constants or experimental input parameters are initially assigned default values (or subsequently induce the program to take a suitable default action) that would be most appropriate for the user in typical problems of interest, were he to fail to define certain parameters explicitly by input. This allows for considerable abbreviation of input, since only essential variables need to be entered to specify execution conditions. At the same time, however, a wide range of variables remain accessible to input specification in case their default values are not acceptable. Input format for NAMELIST entry is very free, and eliminates the possibility of entering numerical data in an incorrect field of columns. Each of the NAMELIST sequences have been given physically descriptive names, and contain variables that specify related parameters for a particular aspect of the analysis.

In order to read data using NAMELIST, input data must be provided in a special form. The first character (column 1) on each card to be

read must be a blank. The second character on the first card (of a group of data cards) must be $ (dollar sign) immediately followed by the NAMELIST name, which must not contain any embedded blanks. The name must be followed by at least one blank, which is followed by a string of data items separated by commas, and the end of a data sequence occurs when another $ is encountered. Any (or all) of the variables included in the NAMELIST group can be entered (without regard to order) as specified input. The form of the data items on an input card is "A = const", where A is the FORTRAN name of a variable or subscripted array, and "const" is an integer, real, complex, or logical constant (or string of constants separated by commas if A is the name of an array). Numerous examples will occur in the sample output to be presented later.

Card input consists of four basic blocks of data to define the molecular kinetic reaction scheme and its rate constants, modifications (if any) for updating an external electron cross section file, comment cards to describe miscellaneous information for reproduction in the output, and experimental input parameters for execution of the analysis.

DATA BLOCK 1

DATA BLOCK 1, whose structure is shown in Table 3.1, occurs only for the initial synthesis of subroutines and generation of data file (on TAPE4) for a new molecular kinetic reaction scheme. The first card is a "header" containing three (10-BCD character) computer words which "name" the new program. They are used as a three-line title on a cover page preceding the output whenever the code is subsequently executed. Following the header card, there is an arbitrarily long se-

AD-A066 155 NORTHROP RESEARCH AND TECHNOLOGY CENTER PALOS VERDES --ETC F/G 20/5
THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSE--ETC(U)
JAN 79 W B LACINA N00014-78-C-0499
UNCLASSIFIED NRTC-79-7R-VOL-1 NL

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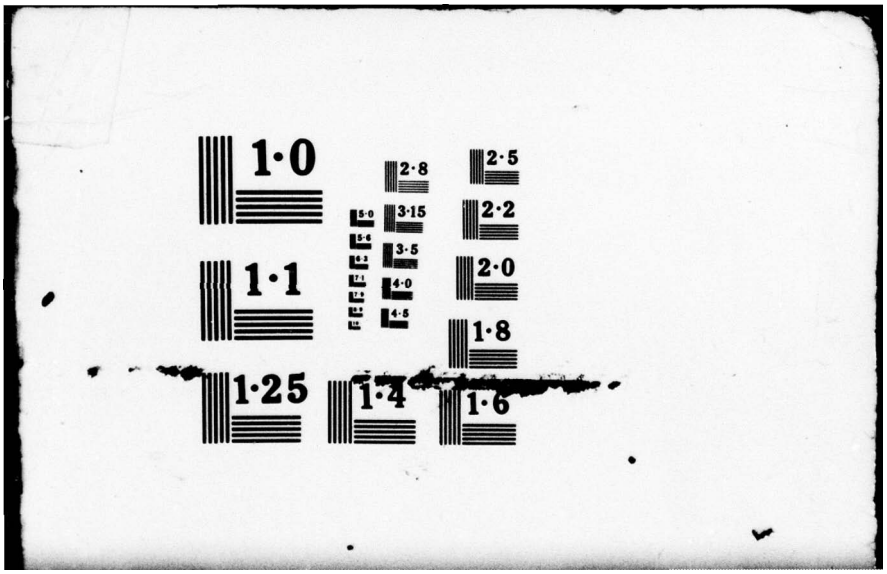

1·0
2·8
2·5
3·15
2·2
3·5
2·0
4·0
1·1
4·5
1·8
1·25
1·4
1·6

Table 3.1: DATA BLOCK 1
(Subroutine Synthesis)

Card 1	TITLE(3) (3A10)
	Header card contains three (10 BCD character) computer words which "name" the program to be synthesized from the reaction scheme which follows.
Card 2 Card 3	Specification of reaction No. 1.
Card 4 Card 5	Specification of reaction No. 2.
⋮	⋮
Card 2n	KINETIC(6) (6A10)
	Symbolic expression, reaction No. n, subject to certain (minimal) restrictions on syntax, and miscellaneous conventions.
Card 2n+1	KF, KR, COMMENT(5) (2E10.3, 5X, 5A10)
	Forward and reverse rate constants for the reaction (with appropriate units), and optional comment or reference for the data.
⋮	

EOF card terminates data package. Number of card pairs is arbitrary, although an error condition results if any dimension storage limit is exceeded.

quence of pairs of cards which define the input reaction scheme, ultimately terminated by an EOF card. (In practice, the length of the reaction queue is limited by the dimension declarator KMAX, and the number of new species encountered during processing is limited to NMAX. KMAX, NMAX, and all other dimension declarators can be easily changed in the main program LASER. If the number of reactions or species exceed the limits, they are ignored, and a diagnostic is issued.)

The first card of a reaction pair consists of a Hollerith string of up to 60 BCD characters, containing an expression of the form

$$A + B + C + \ldots \quad \rightarrow \quad X + Y + Z + \ldots$$

The syntax for the reaction is quite flexible, allowing it to be written just as it would be in usual technical notation. Each side of the reaction may contain up to five species whose names are defined by the first NSIZE (= 10) nonblank characters recognized before a delimiter (+ or $\rightarrow$) is encountered. Embedded blanks are ignored, and certain conventions must be observed:

i) Secondary electrons are denoted by "E", "E-", or "E(-)".

ii) High energy (e^--beam) electrons are denoted by "HE-".

iii) All other charged particles must explicitly exhibit their charge in their name (e.g., "F-", "KR2(+)", "AR(++)", etc.) and multiple charge must be explicit (i.e., "AR(++)" rather than "AR(2+)"). If an ion is positive, the "+" sign must be immediately followed by another "+" or by ")" in order to avoid confusion with the normal usage of "+" in writing reactions.

iv) Numerical coefficient in front of the species not permitted (e.g. A+ B $\rightarrow$ C + C, but not A + B $\rightarrow$ 2C, is allowed).

v) Buffer gases (whose identity is not important) can be denoted by "M" (resulting in a total pressure dependence).

v) Spontaneous emission processes do not have to explicitly include a photon on the right hand side of the reaction unless the process is considered to contribute "noise" to the buildup of an optical field by stimulated amplification, in which case the photon must be included and denoted "HNU".

vi) Stimulated emission or absorption processes are denoted by "RAD". Except for the laser transition involving stimulated emission (in which case "RAD" must appear on both sides of the reaction), "RAD" can occur only on the left hand side.

As they are processed, the reactions of the input kinetic scheme are subjected to several tests to detect errors. Among the possible error conditions encountered are the following:

i) High energy electrons must balance on left and right.

ii) Buffer gas "M" must balance on both sides of equation.

iii) Charge conservation must not be violated.

iv) Reverse processes for spontaneous emission not allowed (i.e., "HNU" must not appear on the left side of a reaction)

v) Stimulated radiation "RAD" must not appear (alone) on the right hand side of a reaction.

vi) Duplicate reactions (even written backward) are ignored.

vii) Detail balance for binary molecular collisions enforced.

viii) For secondary electron collision processes which default to Boltzmann calculation for rate constant, the attached electron cross section data file is searched to verify that appropriate cross section data is available.

ix) Dimension storage (defined by the declarators KMAX, NMAX, and NKMAX) must not be exceeded during program synthesis.

x) Both forward and reverse rate constants zero; reaction is ignored unless it is a secondary electron collision process, in which case rate constants are automatically linked to a coupled Boltzmann analysis.

xi) Reaction syntax unrecognizable.

xii) More than five species on left or right hand side.

If an error is encountered, a diagnostic warning is generated in the edited summary of reaction processing, and the faulty reaction is ignored for the construction of the synthetic subroutines and associated data file. Thus, processing continues uninterrupted throughout the entire input reaction queue, and the final program generated can even be executed unless the user declares the occurrence of such errors to be treated as fatal.

The second card in the pair of cards defining a reaction contains (an initial estimate of) the forward (KF) and reverse (KR) rate constants for the process, and an (optional) 50-character field for comments or a data reference, which will be reproduced in the output. With certain exceptions to be described, both a forward and reverse rate constant are typically provided for each reaction. The units for these rate constants are determined by the structure of the reaction, and are:

cm^2	e^--beam collisions; stimulated emission, absorption
s^{-1}	Spontaneous radiative emission
cm^3/s	Binary collisions
cm^6/s	Three-body interactions
⋮	
cm^{3n}/s	Interaction between (n - 1) species.

The program determines the form of the rate expression, Eq. (2), automatically from the syntax of the reaction, subject to the above conventions, and it is the obligation of the user to insure that input values have the proper units. If KF = 0 (or KR = 0), no translation of the forward (or reverse) reaction term occurs in the synthesized rate subroutines and thus, null operations (containing unneces-

sary multiplications by zero) are eliminated. Rate constants used at the time of synthesis can be changed in subsequent execution, however, so a nonzero value should be used during synthesis for any reaction process (with the exception of secondary electron collisions) which is not to be permanently neglected.

For secondary electron processes, the omission of input rate constants at the time of synthesis automatically results in the linkage of the rate constants to a coupled Boltzmann electron kinetics analysis. Likewise, if a rate constant is explicitly specified, no such linkage occurs. During program generation, for those electron collisions which are to be coupled to a Boltzmann analysis, a search is made to determine if the required electron cross section data is available on the library file attached to TAPE8. If the cross section data is available, 50-character input comment is overridden by a data reference extracted from the library file.

For a binary molecular collision process, the program automatically enforces detail balance between the forward and reverse rate constants (although with no provision for degeneracy factors). The reverse rate is defined to be $KR = KF \exp(-\Delta E/kT)$, where ΔE was given by Eq. (6).

Subsequent modifications of rate constants at the time of execution are permitted, but some rate constants are necessarily inaccessible to such input. If no translation of a reverse process occurred, for example, no future input of that rate constant can contribute. Likewise, if rate constants automatically default to Boltzmann calculations or a detail balance expression, opportunities for input modification cannot be provided. There is one logical exception: if the

analysis has been synthesized with default to Boltzmann electron kinetics, rate constants for secondary electron collisions can be modified (i.e., defined by input) whenever the program is executed under conditions of no electric discharge. If an illegal attempt is made to modify rate constants which are inaccessible to input, a warning diagnostic is issued and the illegal attempt is ignored unless declared to be fatal.

There are three subroutines which are synthesized by translation of the symbolic input reaction scheme into computer-coded equations:

SUBROUTINE DNDT (N, T, NO, NDOT)

This subroutine calculates the instantaneous rates of change of all of the dependent variables in the (first order) system of coupled differential equations (consisting of the master equation (4) and the circuit equations (93) or (94)). Miscellaneous optical (gain, absorption) and electrical parameters (e^--beam voltage drop dV/dx and secondary e^- creation rate S_b, zero-energy e^- creation rate S_o) are also obtained.

Input Parameters:

N	=	Number of equations
T	=	Independent variable, time (s)
NO(I)	=	Vector of dependent variables: I = 1, NTYPE are population densities (cm^{-3}); NTYPE +1 is charge, q (Coul), and NTYPE+2 is current, i (A)

Output Parameters:

NDOT	=	Vector of rates of change of dependent variables: NDOT(I) = d NO(I)/dt.

In addition to the formal calling parameters, there is also communication between DNDT and the main program LASER through labelled COMMON blocks. Since the integration subroutine GEAR is concerned only with the formal calling parameters shown, it need not be explicitly provided with miscellaneous experimental constants and input parameters available in the main program. Likewise, there are certain quantities which are useful by-products of the computations in DNDT such as SB (S_b), S0 (S_o), DVDX (dV/dx), and RATE(I) (the rates of Eq. (2)). Their inclusion in labelled COMMON is convenient for the direct communication of information to the main program LASER.

SUBROUTINE JACOB (N, T, NO, PHI)

This subroutine calculates a Jacobian required by the integration subroutine (GEAR). It computes the (instantaneous values) of the partial derivatives of the rates NDOT(I) with respect to the dependent variables NO(J) at time T. The calculation of the Jacobian is based upon exact expressions obtained from formal differentiation of the rate equations (4) and (93) (or (94)), rather than by numerical differencing. Its availability allows Subroutine GEAR to be utilized with a "method parameter" of MF = 1. Subroutine JACOB and DNDT share the same labelled COMMON blocks with the main program, although no computational results of JACOB are used by LASER itself. The input parameters for JACOB are the same as for DNDT described above.

Output Parameters:

PHI(I, J) = Jacobian array, dimensioned PHI(N, . .) in the calling program, defined by

$$PHI(I, J) = \partial NDOT(I) / \partial NO(J)$$

SUBROUTINE LEVELS (N1, N2, NO)

This subroutine establishes the correspondence between the lower and upper levels of the inelastic electron collision processes, and the species of the molecular kinetics reaction scheme. It provides part of the linkage which couples the Boltzmann analysis to the molecular kinetics. Immediately prior to a call to Subroutine BOLTZ, this subroutine must be called to determine the (instantaneous) values of the lower and upper state population densities.

Input Parameters:

NO(I) = Vector of (instantaneous) population densities (cm^{-3}) for the Ith species in the kinetic scheme.

Output Parameters:

N1(I) = Vector of population densities for the lower states of the Ith inelastic electron collisions.

N2(I) = Vector of population densities for the upper states of the Ith inelastic electron collisions.

Sample output, obtained from synthesis of subroutines DNDT, JACOB, and LEVELS for the KrF laser system, will be presented later. The results of translation of the molecular kinetic scheme into computer-coded FORTRAN equations will be illustrated for several reactions. In addition to reaction translation, there is also generation of internal COMMENT card documentation, which makes the synthesized subroutines completely readable and understandable. They can be used as the source for creation of a BCD UPDATE program library, which can be catalogued and saved, if desired. If the reaction scheme is to be subsequently executed, the binary compilation should be saved.

DATA BLOCK 2

The purpose of DATA BLOCK 2 is to provide updates or modifications to the electron cross section library, attached on TAPE8, immediately prior to execution. The updated file, generated on TAPE9, is then used for execution of the analysis and can be catalogued and saved for future access, if desired. Since the external electron cross section library can be originally constructed by "updating" an empty TAPE8 file with the totality of available data, the format for reading TAPE8, TAPE9, and DATA BLOCK 2 is identical.

DATA BLOCK 2, whose structure is shown in Table 3.2, consists of an arbitrary number of packages of electron cross section data for secondary electron collision processes. The first card of a package contains a 60-BCD character Hollerith field in which the symbolic reaction is specified. The syntax for reactions is quite flexible, and is the same as that described for DATA BLOCK 1 above. Embedded blanks are ignored, and the order of species is not important. Thus, when a search is made for cross section data for an electron collision process encountered in the molecular kinetic scheme, it is not required that the reaction be written identically as it occurs in the external electron data file. Only the content of two reactions compared must be identical; for example, the two reactions

$$KR2(+) + E(-) \rightarrow KR^* + KR$$

and

$$E + KR2(+) \rightarrow KR + KR^*$$

would be recognized to be equivalent. An additional convention is used for specifying momentum transfer cross section for electron collisions with species X:

Table 3.2: DATA BLOCK 2
(Cross Section Update)

Package 1

Package 2

⋮

Package n:

Card 1	KINETIC(6), UNITS, NPTS, MONTH (6A10, F7.3, I3, A10) This card contains a 60-BCD character field for the symbolic specification of an electron collision process. Cross section data entered on subsequent cards is assumed to be expressed in units of UNITS x 10^{-16} cm^2. Default is UNITS = 1 if unspecified. NPTS defines subsequent data format.
Card 2	COMMENT(6) (6A10) 60-BCD character field for comment or data reference. This information is reproduced with requested tabular output of the cross section data, and is automatically extracted as the rate reference in a synthesis program.
Card 3 Card 4	EV, vector of m electron energy values (eV), SIGMA, vector of m corresponding cross section data values. Format for Card 3, 4 is (mEn.0), where m = NPTS and n = 80/NPTS (truncate decimal residue).
⋮	⋮
Card i	Cf. description of Card 3,
Card i+1	Cf. description of Card 4,
⋮	⋮
Card 2k+1	Blank card terminates cross section data for the electron collision process of this package.

⋮

$$E + X \rightarrow E + X$$

Although momentum transfer cross sections must be included in the electron library file, the explicit inclusion of elastic or momentum transfer collisions in the molecular kinetic reaction scheme defined in DATA BLOCK 1 is not required.

The second parameter on the first card, UNITS, is a multiplicative factor to adjust the numerical cross section values, which are assumed to be entered in units of 10^{-16} cm^2. (If UNITS is not specified, it defaults to 1.0.) The third parameter, NPTS, specifies a variable FORMAT (mEn.0), where m = NPTS and n = 80/NPTS (n is an integer obtained from truncation of decimal residue). This FORMAT specifies the number of data fields on subsequent energy and cross section cards to be read from the current package. (If NPTS ≤ 0 or if NPTS > 10, program sets NPTS = 10 by default.) The last parameter, MONTH, is a 10-BCD character specification of the date (e.g., 12/25/78) of cross section submission into the library file. If it is not provided, it is automatically generated by Subroutine UPDATE at the time it is added to the library.

The second card of a package contains a 60-BCD character field for comment or data reference. It is reproduced on requests for output plots or tables of cross sections, and is automatically extracted as the reference for TAPE4 data in the generation of a synthetic program.

Following the first two cards, there is an arbitrary number of card pairs i and i+1, ultimately terminated by a blank card, containing sequences of energies and corresponding cross section values. Card

i contains a sequence of energies (eV), which must be in monotonically ascending order, followed by card (i + 1), which contains the corresponding cross section values (in units of UNITS x 10^{-16} cm^2). The format specification is (mEn.0), as described above. For example, if NPTS = 8, the format would be (8E10.0), defining eight 10-column fields (into which F-numbers could be entered, if desired).

Ultimately, the collection of cross section packages must be terminated by an EOF card.

DATA BLOCK 3

DATA BLOCK 3, shown in Fig. 3.3, consists of an arbitrarily long sequence of comment cards which will be reproduced in the output. It provides a convenient opportunity for documenting the output of an analysis with descriptive remarks. Format is (8A10).

DATA BLOCK 4

DATA BLOCK 4, whose structure is shown in Fig. 3.4, defines experimental parameters, numerical control parameters, fatal error designation, data initialization, and output requests for execution of the synthesized analysis. It consists of six NAMELIST data groups, followed by an arbitrarily long sequence of cards which initialize the energies, molecular weights, and population densities of molecular species. The NAMELIST parameters are defined in Tables 3.5-3.10, which summarize the assumed units and default values. The NAMELIST groups have been constructed to have physically descriptive names, and to contain logically related variables.

The format for the sequence of species cards is (A10, 3E10.3, 10X, A10).

Table 3.3: DATA BLOCK 3
(Descriptive Comments)

Card 1	COMMENT(8)	(8A10)
Card 2	COMMENT(8)	(8A10)
⋮	⋮	
Card n	COMMENT(8)	(8A10)
⋮	⋮	

EOF card termination.

TABLE 3.4: DATA BLOCK 4
(Execution Parameters)

1) $CONTROL ... $

Miscellaneous parameters related to numerical control of the calculations--convergence accuracy, integration order and method, electron energy resolution, interpolation order, fatal declaration of error conditions, frequency of output generation, etc. (Table 3.5).

2) $PARAM ... $

Pressure, temperature, and pulse length (Table 3.6).

3) $OPTICAL ... $

Optical cavity specifications--loss per pass or threshold coefficient, output coupling reflectivity, length, area, solid angle (Table 3.7).

4) $EBEAM ... $

External e^--beam current density, energy, temporal and energy dependent characteristics (Table 3.8).

5) $CIRCUIT ... $

Capacitance, inductance, and resistance of external RLC driving circuit, initial charging voltage, discharge area and electrode separation (Table 3.9).

6) $RATES ... $

(Permissible) modifications to kinetic rate constants for the reaction scheme (Table 3.10).

The above NAMELIST cards are followed by (an arbitrary number of) cards for initialization of species parameters. These cards (which are ultimately terminated by an EOF card) are of the form:

NAME, P, E, MOLWT, OPTION (A10, 3E10.3, 10X, A10)

These cards define the energy E (eV) and molecular weight MOLWT (g/mole) of the species NAME. P is the concentration: if the total pressure is specified by the $PARAM$ card, the P values represent relative fractions. If the total pressure has not been previously specified, the values of P represent partial pressures (Torr), unless their values are > 1.0E 08, in which case they represent actual population densities (cm^{-3}). (Cf. description of PTOT and ATM in Table 3.6.) If OPTION = 4HPLOT, a plot of NAME is generated.

TABLE 3.5 : NAMELIST / CONTROL / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
EMAX	u_{max}	eV	Electron energy range for solution of the Boltzmann equation is $[0, u_{max}]$. Default is EMAX = 20.0. During execution (if EXPAND = .TRUE.), the electron energy range is automatically expanded if certain convergence conditions were not met.
EXPAND			LOGICAL variable which instructs program to automatically expand the electron energy range $[0, u_{max}]$ if the Boltzmann solution did not converge to relative accuracy EPS, or if the power discrepancy exceeds PCT. Default: EXPAND = . F.
MESH	MESH		Number of (equally spaced) intervals into which the electron energy range $[0, u_{max}]$ is subdivided (cf. Eq. (73)). Default is MESH = MGRID. Program does not permit MESH MGRID.
PCT		%	Maximum permissible error in power balance for the electron kinetics analysis; if exceeded (and if EXPAND = .TRUE. was specified), program will attempt to attain better power balance by expanding the range $[0, u_{max}]$. Default: PCT = 5.0.
ITMAX			Maximum number of iterations permitted for the calculation of an electron distribution function $f_o(u)$. If convergence to the required accuracy EPS was not attained, a diagnostic is generated, and program terminates unless EXPAND = .TRUE. Default is ITMAX = 100.

TABLE 3.5: NAMELIST / CONTROL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
TMAX		CP sec	Maximum CP time permitted for calculation of an electron distribution function (cf. description for ITMAX). Default is TMAX = 50.0.
EPS	ϵ		Convergence parameter for solution of the Boltzmann equation (cf. Eq. (92)). Solution for the electron energy distribution proceeds by an iterative technique: as soon as the maximum relative change (over all discrete energies) between two successive iterations is < EPS, convergence is declared. Default is EPS = .001.
TE	T_e	K	Initial electron temperature. Default is TE = TMOL.
IDEG			Degree of (polynomial) interpolation for defining the input electron cross section data over the uniform grid of MESH intervals. Default is IDEG = 2 (quadratic interpolation).
NCYCLE			The total specified pulse length, TPULSE, is subdivided into NCYCLE (equal) intervals of time Δt = TPULSE/NCYCLE. At the discrete points $t_k = k\Delta t$ (k = 0, 1, . . . , NCYCLE) the Boltzmann analysis is updated, and various output (as specified by the option vector IO) is generated. Default: NCYCLE = MAX; if NCYCLE > MAX, program sets NCYCLE = MAX.

TABLE 3.5: NAMELIST /CONTROL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
LIMIT			Number of complete time intervals over which the calculations are carried out. The total pulse length TPULSE is subdivided into NCYCLE (equal) intervals of time Δt = TPULSE/NCYCLE, defining discrete times $t_k = k\Delta t$ ($k = 0, 1, 2, \ldots,$ NCYCLE). The calculations can be restricted to terminate at k = LIMIT. Default is LIMIT = NCYCLE. Program insures that $0 \leq$ LIMIT $\leq$ NCYCLE.
MAXDER			The maximum derivative (order) used in the Gear integration technique. It must be less than eight for the Adams method, and seven for stiff methods. Default is MAXDER = 7. (Cf. comments in Subroutine GEAR.)
METHOD			The specification of method in Subroutine GEAR. METHOD may be 0 (Adams predictor-corrector), 1 (multistep technique suitable for stiff systems), or 2 (same as case 1, except that partial derivatives are computed by numerical differencing). Default is METHOD = 1 (since both the rates $\dot{n}_i$ and the Jacobian $\delta\dot{n}_i/\delta n_j$ are provided by synthesized subroutines). Cf. discussion of Subroutine GEAR.
ETA			Error test for GEAR integration: the step size and order are adjusted to maintain this accuracy. Default: ETA = .001. Cf. comments in Subroutine GEAR.

TABLE 3.5: NAMELIST / CONTROL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
FATAL(I)			Vector of LOGICAL control parameters to specify that certain potential error conditions, if encountered, be treated as fatal: if condition I occurs, and FATAL(I) = .TRUE., execution of the analysis is terminated. (A diagnostic message is generated for each error condition.) Default is FATAL(I) = .FALSE. for conditions I = 1, 2, 3, ... 9; error 10 is automatically declared fatal and is inaccessible to input. Error conditions: 1) Errors were detected in processing the input reaction scheme during subroutine synthesis. Modifications of the reaction scheme, corrections to the reaction syntax, changes in DIMENSION storage, or additions to the electron cross section file may be required. If FATAL(1) = .FALSE., the code ignores defective input. 2) Unrecognized molecular species, which did not occur in the molecular kinetic reaction scheme, were encountered for initialization. If FATAL(2) = .FALSE., such species are assumed to be buffer gases and are included in the total pressure, and as constituents in the electron kinetics analysis (momentum transfer). 3) Not all of the population densities for species present in the synthesized reaction scheme were initialized by input. If FATAL(3) = .FALSE., program initializes these population densities to zero, by default.

TABLE 3.5: NAMELIST / CONTROL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
			4) Not all of the energy levels were specified for the species present in the synthesized reaction scheme. If FATAL(4) = .FALSE., program sets them to zero by default.
			5) Errors were detected in the electron cross section data file (e.g., cross section not defined in the range $[0, u_{max}]$, cross section data not sequenced monotonically in energy, cross section data missing). Default: zero cross section.
			6) Mass, or momentum transfer cross section, for some of the gas species was zero. If FATAL(6) = .FALSE., momentum transfer for these gases is ignored in the electron kinetic calculations.
			7) An attempt was made to modify rate constants which the program considers to be inaccessible by input (e.g., the rate of a reverse process not originally present, a rate defined by detail balance, or a rate for a secondary electron excitation process in an electric discharge). Such an attempt is simply ignored if FATAL(7) = .FALSE.
			8) DIMENSION declarator constants read from TAPE4 (containing the data associated with the synthesized subroutines for a given reaction scheme) do not agree with those defined in the main program LASER. If new storage allocation is greater, there may be no problem. Caution is advised to insure that labeled COMMON blocks agree.

TABLE 3.5: NAMELIST /CONTROL/ Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
			9) Data on TAPE4 contained vectors which exceed maximum allocated DIMENSION storage in the main program, and must, therefore, be truncated upon input loading.
			10) Momentum transfer collision frequency was zero at some point in the electron energy range $[0, u_{max}]$. Since its inverse occurs in the Boltzmann equation, this condition is automatically declared fatal by the program.
IO(I)			Vector of integer constants for specification of output options I, I = 1, 2, 3, . . . , 10. The total pulse duration TPULSE over which the analysis is integrated is subdivided into NCYCLE intervals that define discrete times $t_k = k\Delta t$ (Δt = TPULSE/NCYCLE, k = 0, 1, 2, . . . , LIMIT). At these discrete points, various output options can be requested. IO(I) represents (for I = 1, 2, . . . 7) an integer multiple of the basic cycle index k at which option I is to be generated (options 8, 9, and 10 occur only once, if IO $\neq$ 0). Default is IO(I) = 1 (I = 1, 2, 3, . . . , 10). The output specified by each IO parameter is the following:
			1) Tabular summary of plasma parameters ($\bar{u}$, T_e, D, μ, ϵ_k, ρ, σ, dn_e/dt, ν_i, ν_a, etc. Cf. Fig. 4.12.)
			2) Tabular summary of the electron distribution function $f_o(u)$ as a function of energy u. (Cf. Fig. 4.13.)

TABLE 3.5: NAMELIST / CONTROL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
			3) Logarithmic plot of the normalized electron energy distribution $f_o(u)/f_o(0)$ as a function of energy u (cf. Fig.4.14)
			4) Logarithmic plot of $f_o(u)/f_B(u, T_e)$, where $f_B(u, T_e)$ is the Boltzmann distribution for an effective temperature T_e defined by $T_e = 2\bar{u}/3k$ (in terms of the average energy $\bar{u}$ of the actual distribution $f_o(u)$). (Cf. Fig. 4.15.)
			5) Tabular summary of electrical power partitioning and the forward and reverse excitation rates for all of the inelastic electron collisions included in the Boltzmann analysis. (Cf. Fig. 4.16.)
			Options 1-5 correspond to the output options OUT (5) for Subroutine BOLTZ.
			6) Tabular output of population densities and their rates of change (and effective instantaneous time constants) for all molecular species, and electrical and optical parameters. (Cf. Fig. 4.17.)
			7) Tabular summary of reaction sensitivities (cf. Fig. 4.18.)
			8) Tabular output of raw electron cross section data (cf. Fig. 4.10).
			9) Plots of electron cross section data (cf. Fig. 4.11).
			10) Table of reactions and modifications (if any) of rate constants (cf. Fig. 4.9).

TABLE 3.6 : NAMELIST / PARAM / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
TPULSE		s	Normally, the total pulse length. TPULSE is subdivided into NCYCLE intervals of time over which the molecular kinetic and circuit equations are integrated. At the discrete times $t_k = k\Delta t$ (Δt = TPULSE/NCYCLE, k = 0, 1, 2, . . . , LIMIT), the Boltzmann equation is solved. The combination of NCYCLE, LIMIT, and TPULSE provides flexibility for the joint specification of total integration time and the frequency of electron kinetic updates.
TMOL	T	K	Molecular temperature. Default is TMOL = 300.0.
TE	T_e	K	Initial electron temperature. Default is TE = TMOL.
PTOT		Torr	Total pressure. Default is PTOT = 0.0.
ATM		atm	Total pressure. Default is ATM = 0.0.
			There is a variety of alternative methods for specifying the pressure (or equivalently) the population densities of the species. If PTOT = 0.0, the program sets PTOT = 760. *ATM; then, if PTOT $\neq$ 0.0, input concentrations (to be entered by subsequent input) are assumed to be relative fractions, normalized to a total pressure PTOT. If PTOT = 0.0, it is assumed that input concentrations represent partial pressures (Torr), unless the values are > 1.0E 08, in which case they represent actual population densities (cm^{-3}).

TABLE 3.7: NAMELIST /OPTICAL/ Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
LOSS	γ	%	Single pass loss for intracavity optical elements, exclusive of absorption in the gain medium. Default is LOSS = 0.0 (REAL).
REFLECT	R	%	A simple plane parallel cavity formed by a total reflector and an output coupling mirror of reflectivity R is assumed. The default is REFLECT = 0.0 (high cavity threshold results).
LENGTH	L_g	cm	Length of the active gain medium. If LENGTH $\leq$ 0.0 (REAL), default is LENGTH = 0.01.
CAVITY	L_c	cm	Length of the optical cavity (i.e., mirror separation). The default is CAVITY = LENGTH.
AREA	A	cm^2	Area of the optical output aperture. Default is AREA = 0.0.
OMEGA	Ω	sr	Solid angle subtended by the optical output aperture as viewed from the opposite end of the cavity. Default: OMEGA = A/L_c^2. The buildup of the optical field occurs from amplification (by stimulated emission) of a fraction ($\Omega/4\pi$) of the spontaneous noise. If OMEGA = 0.0, and if the initial value of NO(1) = 0.0, NO(1) will remain zero and there will be no contribution from the stimulated radiation processes in the kinetic scheme. (Cf. Eq. (12), (13), (122), and (123).)

TABLE 3.7: NAMELIST /OPTICAL / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
GAMMA	α_{th}	cm^{-1}	Threshold loss coefficient. Default is GAMMA = 0.0. If GAMMA = 0.0, it is defined by Eq. (124), where γ = LOSS and L_g = LENGTH. If GAMMA $\neq$ 0.0 has been specified, the values of LOSS and REFLECT are ignored.

TABLE 3.8: NAMELIST /EBEAM / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
ENERGY		keV	Electron beam energy (for output reference only).
FACTOR			Multiplicative constant by which all e^--beam cross section values can be increased to account (in a qualitative way) for the larger energy deposition that results from multiple scattering effects in a high pressure gas. Default is FACTOR = 1.0.
UA, UB	u_a, u_b	eV	Cutoff energies to define the (normalized) electron source function s(u) as a square wave (cf. Eq. (111)). Default is UA = UB = 0.0. If UB > EMAX, program sets UB = EMAX. If it were necessary, the program could easily be modified to provide a more complicated shape for s(u).
JB(21), TB(21)			Vectors to define the temporal shape of the e^--beam current density; program automatically renormalizes an input JB(I) to have a maximum value of JBEAM. JB(I) is assumed to be a function of the time TB(I), whose units are UNITS. Specification of JB, TB (which is optional) takes precedence over the alternative methods of defining temporal e^--beam current density described below. (The vector JB(I) is REAL.)
JBEAM	J_b(max)	A/cm^2	Maximum amplitude of e^--beam current density. Default is JBEAM = 0.0. (REAL variable)

TABLE 3.8: NAMELIST /EBEAM / Parameters
(Continued)

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
UNITS			Units of time in which TB(I), TR, TF, TFALL, and TC times are expressed. Default is UNITS = 1.0 E-09 (i. e. nanosecond).
TR	t_r		Rise time. Default is TR = 0.0.
TF	t_f		Fall time. Default is TF = 10,000.0.
TFALL	t_F		Fall time. Default is TFALL = 1.0.
TC	t_c		Cutoff time. Default is TC = 10,000. 0.
			Unless the temporal shape of the e^--beam current density has been explicitly specified in terms of the amplitude J_b = JBEAM and the numerical table [JB(I), TB(I)], it will be defined by $J_b(t) = J_o \exp[-t/t_f][1 - \exp(-t/t_r)], \quad 0 \leqslant t \leqslant t_c$ $J_b(t) = J_b(t_c) \exp[-(t - t_c)/t_F], \quad t_c < t,$ where J_o = JBEAM $(t_r/t_f)[1 + t_f/t_r]^{(1+t_r/t_f)}$, which automatically provides that the maximum amplitude of $J_b(t)$ (which occurs at $t_o = t_r \ln[1 + t_f/t_r]$) shall be J_b(max) = JBEAM.

TABLE 3.9: NAMELIST / CIRCUIT / Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
KVOLT		kV	(REAL variable), giving the initial charging voltage across the capacitor in the external circuit. Default is KVOLT = 0.0.
RESIST	r		External circuit resistance. Default is RESIST = 0.0.
INDUCT	L	H	(REAL variable) representing the external circuit inductance. Default is INDUCT = 0.0.
CAPAC	C	F	External circuit capacitance. Default is CAPAC = 1.0.
AREA	A	cm^2	Discharge electrode area. Default is AREA = 1.0.
DIST	d	cm	Discharge electrode separation. Default is DIST = 1.0.

TABLE 3.10: NAMELIST /RATES/ Parameters

FORTRAN Name	Variable Name	Units	Definition, comments, and default initialization.
KF(I), KR(I)	k_f, k_r		(REAL vectors) representing the forward and reverse rate constants for the Ith reaction in the kinetic scheme. (Units are cm^2, s^{-1}, cm^3/s, cm^6/s, ..., as appropriate.) This NAMELIST permits modification of the initial values of rate constants provided at the time of synthesis of the molecular kinetic subroutines. Program considers some rate constants inaccessible to modification (e.g., rate constants for reverse reactions not originally present, rates related by detail balance, or secondary electron excitation rates in an electric discharge). The default values are the initial rates stored on the data TAPE4.

3.3 Description of Subroutines

The general laser kinetics program LASER requires 16 additional subroutines (in addition to the three which are synthesized, JACOB, DNDT, and LEVELS). An independent program, ELECT, has also been developed specifically for Boltzmann electron kinetics analysis and uses some of the same subroutines. Complete source deck listings for both main programs (LASER and ELECT), as well as for all subroutines used, are included in Vol. II of the present report. Fig. 3.11 summarizes the subroutines required for each program. In this section, some of the more important subroutines will be described. Program ELECT will be described in Sec. 3.4 below.

SUBROUTINE SYNTH(LTAPE, MTAPE, NTAPE, NSCRTCH, NDATA, NSIZE, MAXGAS, GAS, KMAX, NKMAX, LEV1, LEV2, DATE)

This subroutine translates the symbolic reactions of DATA BLOCK 1 into computer-coded equations for the synthesis of subroutines DNDT, JACOB, and LEVELS described in Sec. 3.2. It also compiles the data defining rate constants and references and the structure of the molecular kinetic reaction scheme to generate an associated file on unit NSCRTCH (= 4). Source code is generated as 80-BCD character records on unit MTAPE (= 3), which is compiled for execution. If future execution of a laser kinetics analysis based upon the input reaction scheme is anticipated, the data file on TAPE4 and the source code (and/or its binary compilation) should be catalogued and saved.

Input and output parameters for Subroutine SYNTH are summarized in Table 3.12. Specification of the record content of file NSCRTCH is most easily obtained directly from the listing.

Table 3.11: Deck Structure for Programs LASER and ELECT

Main Program --	LASER	ELECT
Subroutines:		
SYNTH	X	
GEAR	X	
ANALYZE	X	
SHAPE	X	
Synthesized Subroutines:		
JACOB	X	
DNDT	X	
LEVELS	X	
Electron Kinetics Subroutines:		
UPDATE	X	X
PLASMA	X	X
BOLTZ	X	X
Utility Subroutines:		
DEKODE	X	X
SIMEQ	X	X
PLOT	X	X
AXIS	X	X
INTERP	X	X
SIMPSON	X	X
EDITOR	X	X
COVER	X	X
HEADINX	X	X

TABLE3.12: Input Parameters for Subroutine SYNTH

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
LTAPE			File unit LTAPE is used for scratch purposes.
MTAPE, NTAPE			File units for synthesized FORTRAN source code generated. Subroutines DNDT and JACOB are synthesized simultaneously, on NTAPE and MTAPE respectively, as the reaction list of input DATA BLOCK 1 is processed. Subroutine LEVELS is then generated on NTAPE. Finally, NTAPE is copied onto MTAPE. At the termination of synthesis, MTAPE then contains three consecutive subroutines, JACOB, DNDT, and LEVELS.
NSCRTCH			File unit on which reaction data is written. TAPE NSCRTCH must be saved along with the FORTRAN source code if future execution of the synthetic program is anticipated.
NDATA			File unit containing the electron cross section library.
NSIZE			In the symbolic reaction scheme, the first NSIZE characters of a species name are recognized and all others ignored. NSIZE $\leq$ 10.
MAXGAS			Dimension declarator in calling program for maximum number of different species. Program automatically reserves 1 and 2 for radiation and secondary electrons, respectively.
KMAX			Dimension declarator in calling program for maximum number of reactions in the molecular kinetic scheme.

TABLE 3.12: Input Parameters for Subroutine SYNTH
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
NKMAX			Dimension declarator in calling program for the maximum number of secondary electron collision processes in the molecular kinetic reaction scheme.
GAS, LEV1, LEV2			Integer scratch arrays provided by the calling program for species names and identification of lower and upper excited states in electron collision processes.
DATE			(Integer) variable containing Hollerith specification of the date (e.g., 10H 10/17/78) of program generation.

The main purpose of Subroutine SYNTH is to dissect the syntax of (certain types of) symbolic reactions, and to translate the fundamental information content into computer-coded equations. It has been "taught" to recognize the meaning of a reasonably general class of expressions as well as to detect the occurrence of miscellaneous error conditions. If necessary, the user could extend its translation or error detection capabilities, and is at liberty to specify in detail the structure of the synthesized subroutines. For example, the present techniques could be extended in such a way that an encountered "species" such as "XYZ(I)" would be recognized as a representative member of a manifold of vibrational levels, and the reaction syntax,

$$XYZ(I) + AB(J) \rightarrow XYZ(I-1) + AB(J+1)$$

could be interpreted to be a class of vibrational-vibrational exchange collisions to be translated into appropriate DO-LOOPS over I, J in the generated FORTRAN source code. The translation of reactions performed by the present version of SYNTH is best illustrated by examples and is therefore postponed until Sec. 4, where results for the KrF laser system are described.

SUBROUTINE GEAR (N, T, Y, SAVE, H, HMIN, HMAX, EPS, MF, YMAX, ERROR, KFLAG, JSTART, MAXDER, M, PW)

This subroutine was modified from "Subroutine DIFSUB", which appears in the work of Gear[6] on numerical initial value problems in ordinary differential equations. (Cf. Ref. 6, pp. 155-166.) It is a subroutine for integration of a "stiff" system of coupled, first order, differential equations with the capability for automatic control of the step size and order of predictor and corrector. The replacement of "MATINV" discussed in the "Note to Program" (cf. p. 158, Ref. 6)

has been implemented by the use of Subroutine SIMEQ to avoid the initial calculation of a matrix inverse, followed by successive pre-multiplications of a sequence of vectors with that inverse. Input and output parameters are completely described by COMMENT cards in the listing in Vol. II.

SUBROUTINE UPDATE (INFILE, NTAPE, NSCRTCH, LIST, DATE)

This subroutine searches two input data sources, a file unit INFILE and/or card input, to generate an updated electron cross section data library on unit NTAPE. (LASER uses INFILE = 8, NTAPE = 9.) The updated file on NTAPE contains all of the data of INFILE, modified with the additions or revisions defined by card input. A complete cross section data package (cf. Table 3.2 and the discussion of DATA BLOCK 2) must be provided for the initial addition, or subsequent modification, of any collision process. NSCRTCH is a scratch file. If LIST = .TRUE., the contents of the updated file NTAPE are generated in output. DATE is an (INTEGER) variable containing a 10-BCD Hollerith date (e.g. 10H 10/23/75).

SUBROUTINE PLASMA (NDATA, MAX, MESH, LHS, RHS, PROCESS, EV, F, G, Q, U0, UM, NTYPE, NAME, MISSING, ERROR, OUTSIDE, IDEG, OUT)

This subroutine scans the electron cross section library, on file unit NDATA, to extract the cross section data for input reaction defined by LHS and RHS, integer variables generated by Subroutine DEKODE which uniquely specify the left and right hand collision species. The reaction is also described by PROCESS (a 4-vector), containing a 40 BCD character (possibly abbreviated) symbolic expression of the re-

action (used for output purposes only). Input and output parameters are fully described in COMMENT cards in the listing.

SUBROUTINE BOLTZ (MAX, MESH, NK, GAS, FRACT, MIX, NMOL, TMOL, ITMAX, TMAX, EPS, KAPTION, DATE, OUT, EVCM, NE, PROCESS, U, N1, N2, NEL, S, SBEAM, SOURCE, X, XQ, QM, F, G, A, B, VSIG, POWER, PCOLL, DISCH, DEPOSIT, MU, D, EK, AMPS, UBAR, TE, CONVRGE, PBAL)

This subroutine implements the numerical solution of the Boltzmann equation for the electron energy distribution, using the computational algorithms described in detail in Sec. 2.3. Input parameters are described in Table 3.13, and output parameters in Table 3.14. Extensive internal COMMENT card documentation is also included in the listing, given in Vol. II.

SUBROUTINE DEKODE (NAME, IMAGE, LHS, RHS, LABEL, GAS, NSIZE, NTYPE, LONG)

This subroutine dissects the symbolic reaction equations to determine the species on the left and right hand sides. A Hollerith specification of the reaction is provided as an input vector, IMAGE(I), I = 1, LONG. Embedded blanks are permitted, and up to NSIZE characters of a species name are recognized and the rest ignored (NSIZE $\leq$ 10). The vector NAME provided by the calling program contains the names of NTYPE species which have previously been encountered and stored; if additional new species are recognized in the reaction defined by IMAGE, the vector NAME is automatically extended to include them, and NTYPE is increased appropriately upon return. GAS(J,K) is an (INTEGER) array containing the (10 BCD character) Hollerith name of the Jth species (J = 1, 5) on the left (K = 1) and right (K = 2) side

TABLE 3.13: Input Parameters to Subroutine BOLTZ

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
MAX			DIMENSION declarator, defined for various vectors and arrays in the calling program (S, X, XQ, QM, F, G, A, B).
MESH	MESH		Number of (equal) subdivisions into which the electron energy interval $[0, u_{max}]$ is partitioned (Eq. (73)). MESH + 1 $\leqslant$ MAX
NK			Number of inelastic secondary electron collision processes included in the analysis (labeled by α in the sum of Eq. (41)).
GAS(K)			Names (containing up to 10 BCD characters) of the Kth gas in the mixture (declared INTEGER by calling program).
FRACT(K)			Relative fraction of the Kth gas in the mixture. BOLTZ automatically normalizes: $\sum_K \text{FRACT(K)} = 1.$
MIX			Number of gases in the mixture.
			MIX, GAS(K), and FRACT(K) are communicated for output labeling only, and can be restricted, as desired, by the calling program (e.g., limited to the major constituents). The concentrations are automatically sorted into descending order.

TABLE 3.13: Input Parameters to Subroutine BOLTZ
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
NMOL	N	cm^{-3}	Total neutral particle density.
TMOL	T	K	Molecular temperature.
ITMAX			Maximum number of iterations permitted for attainment of convergence of electron energy distribution. If ITMAX $\leqslant$ 0, BOLTZ omits solution of Boltzmann equation, and transfers control directly to calculation of plasma parameters based upon the input distribution function F(I).
TMAX		CP sec	Maximum CP time allowed for calculation of the electron energy distribution function.
EPS	ϵ		Convergence parameter: maximum relative change (over all energies) of the electron distribution between two successive iterations (cf. Eq. (92)).
KAPTION			KAPTION(4) contains a 40 BCD character title for output captions.
DATE			INTEGER Variable, containing the date (e. g., 12/15/78).

TABLE 3.13: Input Parameters to Subroutine BOLTZ
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
OUT(5)			LOGICAL vector of output requests: if OUT(I) = .TRUE., the following output is generated: 1) Table of plasma parameters ($\bar{u}$, T_e, D, μ, ϵ_k, v_d, ρ, σ, dn_e/dt, ν_{mom}, ν_i, ν_a, etc. Cf. Figure 4.12.) 2) Table of normalized electron distribution function $f_o(u)$ as a function of energy u. (Cf. Fig. 4.13.) 3) Plot of $f_o(u)/f_o(0)$ as a function of u (cf. Fig. 4.14). 4) (Logarithmic) plot of the relative distribution $f_o(u)/f_B(u)$ where $f_B(u)$ is the Maxwell distribution at the effective electron temperature T_e defined for the actual distribution $f_o(u)$. (Cf. Fig. 4.15.) 5) Table of secondary electron excitation rates, rates of electron creation and loss, and power partitioning into all of the elastic and inelastic scattering mechanisms. Summary of electrical power balance. (Cf. Fig. 4.16.)
EVCM	E	V/cm	Applied electric field.
NE	n_e	cm^{-3}	Secondary electron density.

TABLE 3.13: Input Parameters to Subroutine BOLTZ
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
PROCESS			Array, dimensioned PROCESS(4, **) in the calling program, containing four words per column which provide a 40 BCD character specification of each of the inelastic collision processes (i. e., the symbolic reaction equation) for output.
U(J)	u_α	eV	Vector containing the inelastic energy loss for the Jth electron collision process.
N1(J)	N_α	cm^{-3}	Vector containing the neutral particle density of the initial state of the Jth inelastic electron collision process.
N2(J)	N_α^*	cm^{-3}	Vector containing the neutral particle density of the final state of the Jth inelastic electron collision process.
NEL(J)			(Net) number of electrons (right hand side - left hand side) for the Jth electron collision process. (For reactions which conserve electrons, NEL = 0; for secondary ionization, NEL = 1; for attachment or recombination, NEL = -1, etc.)
S(I)	s(u)	eV^{-1}	Normalized e^--beam source function at energy $u_I = (I-1)\Delta u$. (Cf. Eq. (106), (107), and (111).)
SBEAM	S_b	$cm^{-3}s^{-1}$	Total rate of creation by an external source of ionization (e. g. e^--beam) of electrons at positive energies ($u > 0$).

TABLE 3.13: Input Parameters for Subroutine BOLTZ
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
SOURCE	S_o	$cm^{-3}s^{-1}$	Total rate of creation of secondary electrons at zero energy from external reactions (i.e. excluding secondary ionization) Cf. Eq. (39), (68), and (109) for the definition of the external electron source function.
X(I)	u_i	eV	Vector of electron energies, X(I) = (I - 1)Δu (cf. Eq. (73)).
XQ(I, J)		$eVcm^2$	Array of quantities, dimensioned XQ(MAX, **) in the calling program, defined by XQ(I, J) = X(I)Q_J(I), where Q_J(I) is the Jth inelastic cross section at energy X(I).
QM(I, K)			Array (containing two column vectors) dimensioned QM(MAX, 2) in the calling program, defined by
		eVcm	$QM(I,1) = u_i^+ / \langle N Q_m(u_i^+) \rangle$,
		eV^2/cm	$QM(I,2) = (u_i^+)^2 \langle (2m/M) N Q_m(u_i^+) \rangle$,
			where $u_i^+ = u_i + \Delta u/2$ (Cf. Eq. (32), (75), (77), and (78).)
G, A, B			Scratch vectors, dimensioned G(MAX), A(MAX,3), and B(MAX) in the calling program (Cf. OUTPUT description).

TABLE 3.13: Input Parameters to Subroutine BOLTZ
(Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
F(I)	f_i	$eV^{-3/2}$	F(I) = $f_i = f_o(u_i)$ is, upon input, an initial guess vector (dimensioned F(MAX) in the calling program) for the electron energy distribution (which need not be normalized) defined over the energy grid X(I). Numerical solution of the Boltzmann equation proceeds by an iterative scheme initiated with the input guess; if ITMAX $\leqslant$ 0, plasma parameters can be calculated for the specified input vector F(I).

TABLE 3.14: Output Parameters for Subroutine BOLTZ

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
VSIG	$\langle v Q_{\pm\alpha} \rangle$	cm^3/s	Array, dimensioned VSIG(2, **) in the calling program, containing the forward and reverse electron excitation rates for the inelastic collision processes: (Cf. Eq. (49).) VSIG(1, J) = $\langle v Q_J(u) \rangle$, VSIG(2, J) = $\langle v Q_{-J}(u) \rangle$, Jth collision process

TABLE 3.14: Output Parameters for Subroutine BOLTZ (Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
POWER(J)	P_α	W/cm^3 or W/elect	(Net) power density partitioned into the Jth inelastic process (accounting for forward and reverse collisions, as required). If NEL = 0, $$P_\alpha = n_e e u_\alpha [N_\alpha \langle v Q_\alpha(u)\rangle - N_\alpha^* \langle v Q_{-\alpha}(u)\rangle].$$ If NEL > 0, the term with N_α^* does not appear; if NEL < 0, the appropriate expression is $$P_\alpha = n_e e(2e/m)^{1/2} N_\alpha \int_0^\infty du\, u^2 f_o(u) Q_\alpha(u).$$ (Cf. Eq. (61), (62), (67), and accompanying discussion.) If $n_e = 0$, plasma parameters are all independent of electron density, and calculation is assumed to be per electron (i.e. units of W/electron).
PCOLL	$\sum_\alpha P_\alpha$	W/cm^3 or W/elect	Total electrical power density partitioned into inelastic scattering processes: $$PCOLL = \sum_J POWER(J)$$

TABLE 3.14: Output Parameters for Subroutine BOLTZ (Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
ELASTIC	P_e	W/cm^3 or W/elect	Electrical power density converted to elastic heating of the molecular gas: $$P_e = en_e(2e/m)^{1/2} \int_0^\infty du\, u^2 \langle (2m/M)NQ_m \rangle [f_o + \frac{kT}{e}\frac{df_o}{du}]$$ (Cf. Eq.(67).) If $n_e = 0$, subroutine calculates P_e/n_e (power per electron).
DEDT		W/cm^3 or W/elect	Rate of change of energy density of stored electron kinetic energy: $$DEDT = e\bar{u}\, dn_e/dt$$
DISCH		W/cm^3 or W/elect	Electrical power density into the gas from the electric discharge: $$DISCH = en_e \mu E^2$$
DEPOSIT		W/cm^3 or W/elect	Power density deposited as electron kinetic energy by external source of ionization: (Cf. Eq. (67), (71), and (110).) $$DEPOSIT = e \langle U^+ \rangle S_b$$

TABLE 3.14: Output Parameters for Subroutine BOLTZ (Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
			The units for all of the power density terms described above are W/cm^3 if the input value NE is not zero. If $n_e = 0$, the calculations correspond to setting $n_e = 1$ (i.e. parameters are calculated per electron), and corresponding units become W/electron.
DNEDT	dn_e/dt	$cm^{-3}s^{-1}$	Self-consistently calculated value of the rate of change of the secondary electron density (Cf. Eq. (56) and accompanying discussion.) Upon input, DNEDT can be entered as an initial estimate of dn_e/dt, which is then determined self-consistently in an iterative loop.
DLNEDT	$dn_e/dt/n_e$	s^{-1}	Logarithmic derivative of electron density: $\text{DLNEDT} = d/dt(\ln n_e) = dn_e/dt/n_e$
IONIZE	ν_i	s^{-1}	Total secondary ionization frequency.
ATTACH	ν_a	s^{-1}	Attachment (and recombination) frequency.
VD	v_d	cm/s	Drift velocity: $v_d = \mu E$ (Cf. Eq. (50) and (55).)
MU	μ	cm^2/Vs	Electron mobility (cf. Eq. (50)).

TABLE 3.14: Output Parameters for Subroutine BOLTZ (Continued)

FORTRAN Name	Variable Name	Units	Description, comments, and references to the theoretical discussion in the text.
EK	ϵ_k	eV	Characteristic energy (cf. Eq. (54)).
AMPS	J/n_e	A cm	Electric discharge current density, per unit electron density: $$\text{AMPS} = J/n_e = ev_d.$$
UBAR	$\bar{u}$	eV	Average electron energy (cf. Eq. (52)).
TE	T_e	K	Effective electron temperature: $\bar{u} = (3/2)kT_e$ (Eq. (53)).
CONVRGE			LOGICAL variable defining (if .TRUE.) successful convergence of the iterative solution to the Boltzmann equation (41).
PBAL		%	If the Boltzmann equation is correctly solved, the equation (67) for power balance will be satisfied, except for a possible discrepancy ΔP resulting from numerical errors: $$\text{PBAL} = 100\ \Delta P/(\text{DISCH} + \text{DEPOSIT}).$$
F, G, B	f_i	$eV^{-3/2}$	Upon successful convergence, F(I) is the normalized electron distribution; $G(I) = F(I)/F(1) = f_o(u)/f_o(0)$; and $B(I) = f_o(u)/f_B(u,T_e)$, where $f_B(u,T_e)$ is the Boltzmann distribution at the effective temperature T_e.

of the reaction, and LABEL(J, K) are the integer labels for GAS(J,K) which correspond to the sequential ordering of the species in the vector NAME(I), I = 1, NTYPE. If there are less than the five species permitted on the left (or right) hand side, the default value for arrays GAS and LABEL are 1H (blank) and 0, respectively. Further details concerning reaction syntax were given in the discussion of DATA BLOCK 1 above.

In order to make possible a simple comparison between two sequences of collision partners (which may be only rearranged), Subroutine DEKODE also generates INTEGER variables LHS and RHS to uniquely describe the left and right hand side of the reaction. If a sequence of collision partners contains species defined by the integer indices ℓ_J, two sums are defined

$$L = \sum_J \ell_J ,$$

$$LSQ = \sum_J \ell_J^2 .$$

L and LSQ are then encoded into an (INTEGER) variable, with format (I4, I6), to define an "identifier" (i.e., LHS or RHS), which is invariant to a permutation of the component species ℓ_J and believed to be unique, for all practical purposes. The identifiers LHS and RHS are used as Hollerith variables, and contain numbers with no physical significance.

LASER initializes the vector NAME(I) in such a way that I = 1 and 2 are reserved for radiation and secondary electrons, respectively.

SUBROUTINE SIMEQ (A, M, N, N1, SING)

The purpose of this subroutine is to solve an N x N system of simultaneous equations of the form

$$\sum_{J} A(I, J)\, X(J) = B(I),$$

where I = 1, 2, 3, . . . , N. Input consists of putting the N x N matrix of coefficients into the upper left hand box of the array A, which is dimensioned A(M,NCOL) in the calling program. N1 different B-vectors can be specified, stored in successive columns to the right of the N x N matrix (cf. Fig. 3.2). ($M \geq N$, and $N+N1 \leq NCOL$.) Upon output, the coefficients in the upper left hand N x N box are destroyed, and the solution vectors X replace the corresponding input vectors B. That is, the N1 column vectors B of length N form an N x N1 array B, which is transformed to $A^{-1}B$ upon output. In particular, if N B-vectors are chosen to form the unit matrix, output will consist of the inverse A^{-1}. SING is a logical variable which is returned .FALSE. unless the coefficient matrix is singular.

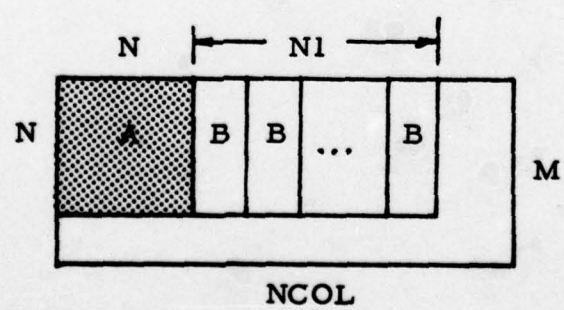


Fig. 3.2: Input array structure for SIMEQ.

SUBROUTINE PLOT (MM, MP, MULT, Y, Y0, DY, X, X0, DX, SCALEX, SCALEY, SAME, CLEAR, CENTER, NAME, NP, IP)

This subroutine generates linear, logarithmic, or semilogarithmic plots for NP vectors ($NP \leq 10$), Y(I, J), J = 1, 2, . . . , NP. A variety of options exist for automatic scaling of the X- and Y-axes to convenient (integer) tick mark divisions, for simultaneous or independent scaling of data, and for output labeling. Extensive documentation, definition of input parameters, and instructions for usage can be found in the COMMENT cards in the listing.

SUBROUTINE AXIS (SCALE, XMAX, XMIN, X0, DX, XDC)

This subroutine is used for automatic scaling of axes for Subroutine PLOT. XMAX and XMIN are input values of the maximum and minimum values of the vector to be scaled. The range of values (XMAX - XMIN) is to be spanned by a convenient origin X0 and integer tick-mark spacing DX. XDC is set equal to zero unless the range 10 DX < X0/1000, in which case XDC is set equal to X0, X0 is reset to zero, and XMAX and XMIN are reduced by an amount XDC. Thus, XDC corresponds to a "dc baseline" that is returned nonzero whenever the range of the plot is very small relative to the absolute magnitude of the values themselves.

SUBROUTINE INTERP (IDEG, XP, YP, X, Y, MULT, N)

This subroutine will interpolate a vector Y(I), assumed to be a function of a vector X(I), to produce that value YP which corresponds to

the value XP. IDEG = 1, 2, 3, ... specifies linear, quadratic, ... interpolation. The vectors X(I) and Y(I) provided by the calling program are sampled with a repetition index MULT, with N points defined at I = 1, (1+MULT), ... (1+(N-1)MULT) used. (Normal usage is MULT = 1.) Values of X(I) must be in ascending order. XP need not lie within the range of the vector X(I), but if it falls outside, linear interpolation is automatically used.

SUBROUTINE SIMPSON (F, M, H, ANS)

This subroutine integrates (Simpson method) a function defined as a vector F over N = 2M subintervals of width H, with result ANS.

SUBROUTINE EDITOR (INPUT, LIST)

This subroutine reads 80-BCD character records on unit INPUT to an EOF and rewrites them onto TAPE5, creating an effective card input file on TAPE5 each time a data block is processed. LIST = .TRUE. produces an output "playback" listing of the input card images, thus providing an exact output record of the input card decks.

SUBROUTINE COVER (TITLE, NPAGE)

NPAGE identical cover pages, each containing a three-line block-lettered title defined by TITLE(3), are generated for output.

SUBROUTINE HEADINX (JSYMB, JPAGE, MESSAGE)

This subroutine converts a 10-character phrase defined by an input vector MESSAGE(10) to block-letters. Refer to listing for usage.

3.4 Boltzmann Analysis Program

An independent program (ELECT) has been developed, concurrently with LASER, for Boltzmann analysis of a specified gas mixture and (sequence of) E/N values. As Table 3.11 shows, these two programs share the same subroutine file for those computational tasks which are common to both. Furthermore, the structure of the external electron cross section library is compatible for use with either program (cf. description of DATA BLOCK 2 in Sec. 3.2). A complete listing of ELECT, documented by COMMENT cards, is given in Vol. II.

Input deck structure for execution of the analysis consists of a set of data blocks, each terminated by an EOF (7/8/9 card), as shown in Fig. 3.3. The first data block is identical to DATA BLOCK 2 (for an update of the electron cross sections) described in Sec. 3.2. The second, DATA BLOCK A, consists of an (optional) sequence of symbolic reactions (60 BCD characters) to specify a set of secondary electron collisions to which the Boltzmann kinetics analysis will be restricted. If none are specified, the program will automatically use the available electron cross section library and retain all collision processes which involve any of the species which are subsequently initialized. DATA BLOCK A is followed by an arbitrary number of data blocks containing physical parameters for execution. The syntax for DATA BLOCK A is the same as that described previously for the reactions in DATA BLOCK 1 and DATA BLOCK 2.

The structure of DATA BLOCK B containing execution parameters is shown in Table 3.15. NAMELIST entry with suitable default initialization is used for input of numerical control parameters, physical data, and initialization of the components of the mixture.

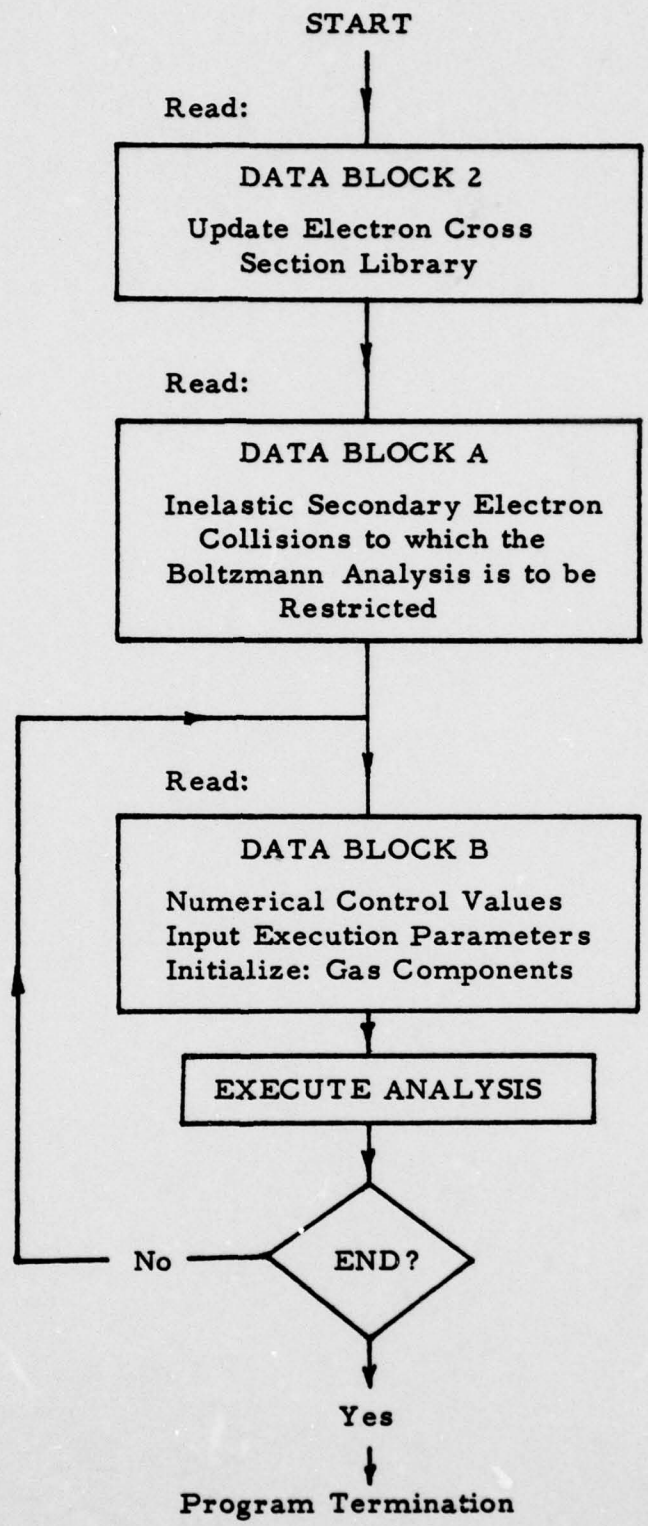


Fig. 3.3: Input data deck structure for Program ELECT.

TABLE 3.15: DATA BLOCK B
(Boltzmann Execution Parameters)

---

1) $CONTROL ... $

Miscellaneous parameters related to numerical control of the calculations--convergence accuracy, energy resolution, interpolation order, output options, etc.

2) $PARAM ... $

Pressure, temperature, and E/N values

3) $SOURCE ... $

Parameters related to the magnitudes (S_o and S_b) and energy dependence of an external ionization source function (e.g., e^--beam).

4) Arbitrarily long package of species cards for specification of concentrations, energies, and molecular weights

---

1) NAME, P, E, MOLWT (A10, 3E10.3)

2) NAME, P, E, MOLWT

⋮

i) NAME, P, E, MOLWT

⋮

These cards define the energy E (eV), molecular weight MOLWT (g/mole), and concentration P of the species NAME. If the total pressure has been specified by the $PARAM ... $ entry, the P values represent partial fractions; if not, they represent partial pressures (Torr) unless their values are > 1.0E 08, in which case they represent actual population densities (cm^{-3}).

3.5 Execution Control Cards

In the present section, some illustrative examples of the typical control card sequences required for execution of Program LASER and ELECT will be given. Obviously, job control language is characterized by considerable variations between different computer systems, as well as by fairly rapid evolutionary changes for any given system. Since the present programs were developed for execution under Extended Fortran Compilation on the CDC 6000 and CYBER Series of computers, the control card syntax appropriate for that system will be illustrated.

First of all, it is convenient to create, from the FORTRAN source deck, a BCD UPDATE program library for convenience in modifying the program if necessary. Fig. 3.4a illustrates the creation of such a file, which is given the name "LASERBCD" and catalogued and saved for future access. Furthermore, the binary compilation file has been catalogued and saved as "LASERFTN" for future execution of the code. A similar sequence of operations for Program ELECT is shown in Fig. 3.4b.

Assuming that the user finds the present version of the source code satisfactory, it can be used for synthesis and execution of analysis with the control cards and deck structure shown in Fig. 3.5. The input reaction scheme specified in DATA BLOCK 1 is translated into FORTRAN subroutines on TAPE3, which is subsequently used as the source for creation of a BCD UPDATE program library that is catalogued and saved with the name "KRFBCD". The file of data associated with the reaction scheme (created on TAPE4) is catalogued and saved with the name "KRFDATA". Two binary compilation files are

```
FILES,TXXX,IOXXX,PX.
USER(ABC,XYZ)
PROJECT(*NNN*NAME)
REQUEST,NEWPL,*PF.
REQUEST,LGO,*PF.
UPDATE(N,F)
CATALOG(NEWPL,LASERBCD,ID=XXX)
FTN(I=COMPILE,R=3)
CATALOG(LGO,LASERFTN,ID=XXX)
7/8/9 CARD
*DECK,LASER
      PROGRAM LASER (...)
                .
                .
                .
*DECK,SYNTH
      SUBROUTINE SYNTH (...)
                .
                .
                .
*DECK,HEADINX
      SUBROUTINE HEADINX (...)
                .
                .
                .
7/8/9 CARD
6/7/8/9 CARD
```

FORTRAN SOURCE PROGRAM

(a)

```
FILES,TXXX,IOXXX,PX.
USER(ABC,XYZ)
PROJECT(*NNN*NAME)
REQUEST,NEWPL,*PF.
REQUEST,LGO,*PF.
UPDATE(N,F)
CATALOG(NEWPL,BOLTZBCD,ID=XXX)
FTN(I=COMPILE,R=3)
CATALOG(LGO,BOLTZFTN,ID=XXX)
7/8/9 CARD
*DECK,ELECT
      PROGRAM ELECT (... )
                .
                .
                .
*DECK,UPDATE
      SUBROUTINE UPDATE (...)
                .
                .
                .
*DECK,HEADINX
      SUBROUTINE HEADINX (...)
                .
                .
                .
7/8/9 CARD
6/7/8/9 CARD
```

(b)

Fig. 3.4: Creation of a BCD UPDATE program library from the FORTRAN source deck, and a binary compilation file for program execution.

```
Control Cards
SYNTH,TXXX,IOXXX,PX.
USER(ABC,XYZ)
PROJECT(*NNN*NAME)
REQUEST,NEWPL,*PF.
REQUEST,BIN,*PF.
REQUEST,BINARY,*PF.
REQUEST,TAPE4,*PF.
REQUEST,TAPE9,*PF.
ATTACH(LGO,LASERFTN,ID=XXX)
LDSET(PRESET=INDEF)
LGO.
UPDATE(N,I=TAPE3)
CATALOG(NEWPL,KRFBCD,ID=XXX)
FTN(I,B=BIN,R=3,EL=F)
CATALOG(BIN,KRFBIN,ID=XXX)
COPYL(LGO,BIN,BINARY,,AR)
CATALOG(BINARY,KRFLASER,ID=XXX)
CATALOG(TAPE4,KRFDATA,ID=XXX)
LDSET(PRESET=INDEF)
BINARY(PL=25000)
CATALOG(TAPE9,CROSSSECTIONS,ID=XXX)
7/8/9 CARD
HEADER CARD
A + B → C + D
   KF      KR          REFERENCE
                  .
                  .
                  .
DATA BLOCK 1
      ARBITRARILY LONG SEQUENCE OF REACTIONS
                  .
                  .
                  .
7/8/9 CARD
                  .
                  .
                  .
DATA BLOCK 2
      STACKED E- CROSS SECTION PACKAGES
      (ARBITRARILY MANY ARE PERMITTED.)
                  .
                  .
                  .
7/8/9 CARD
DATA BLOCK 3
      COMMENT CARDS
                  .
                  .
                  .
7/8/9 CARD
 $CONTROL ... $
 $PARAM ... $
 $OPTICAL ... $
 $EBEAM ... $
                  .
                  .
                  .
6/7/8/9 CARD
```

Fig. 3.5: Synthesis of program defined by input reaction scheme, catalogue of permanent files, and execution of analysis.

created. The compilation of the synthesized subroutines (i.e. JACOB, DNDT, and LEVELS) for the input reaction scheme is catalogued as "KRFBIN". The complete binary file (containing the main program LASER, all of its subroutines, and the subroutines just synthesized) is catalogued as "KRFLASER". The analysis which follows (defined by DATA BLOCK 2, 3, 4) is then executed under the binary file KRF-LASER. Note that no electron cross section library has been attached on TAPE8; the first time the program is run, DATA BLOCK 2 must contain card input of all available electron cross section data for the initial creation of such a library on TAPE9, which is shown catalogued as CROSSSECTIONS. For all future execution of an analysis based upon the input reaction scheme, the binary file KRFLASER can be used, and CROSSSECTIONS can be attached to TAPE8, as shown in Fig. 3.6.

If it is desired to modify the present version of the program, this can easily be done using UPDATE procedures. If these modifications include (but are not necessarily limited to) changes in subroutine SYNTH, the control cards and deck structure shown in Fig. 3.7 are appropriate. The three previously created permanent files LASERBCD, LASERFTN, and CROSSSECTIONS are attached as designated. Modified subroutines are compiled and the old versions replaced by the new using the COPYL command. The new binary compilation file is catalogued (as LASERFTN) and the old one purged. Program LASER is then executed in its updated version, according to the input of DATA BLOCK 1, 2, 3, and 4. Revisions or additions to the electron cross section data of DATA BLOCK 2 are incorporated permanently by cataloging the updated file on TAPE9 as "CROSSSECTIONS" and purging the initial file that was attached to TAPE8. If modifications to program LASER do not involve subroutine SYNTH, and it is only desired to make cer-

```
                 LASER,TXXX,IOXXX,PX.
                 USER(ABC,XYZ)
Control          PROJECT(*NNN*NAME)
Cards            ATTACH(BIN,LASERFTN,ID=XXX)
                 ATTACH(BINARY,KRFBIN,ID=XXX)
                 ATTACH(TAPE4,KRFDATA,ID=XXX)
                 ATTACH(TAPE8,CROSSSECTIONS,ID=XXX)
                 LOAD(BINARY)
                 LDSET(PRESET=INDEF)
                 BIN(PL=25000)
                 7/8/9 CARD
DATA                  STACKED E- CROSS SECTION PACKAGES
BLOCK 2               (ARBITRARILY MANY ARE PERMITTED.)
                                 .
                                 .
                                 .
                 7/8/9 CARD
DATA                  COMMENT CARDS
BLOCK 3                          .
                                 .
                                 .
                 7/8/9 CARD
                  $CONTROL ... $
                  $PARAM ... $
DATA              $OPTICAL ... $
                  $EBEAM ... $
BLOCK 4           $CIRCUIT ... $
                  $RATES ... $
                                 .
                                 .
                                 .
                 7/8/9 CARD
                 6/7/8/9 CARD


                 LASER,TXXX,IOXXX,PX.
                 USER(ABC,XYZ)
Alternate        PROJECT(*NNN*NAME)
Control          ATTACH(BINARY,KRFLASER,ID=XXX)
Cards            ATTACH(TAPE4,KRFDATA,ID=XXX)
                 ATTACH(TAPE8,CROSSSECTIONS,ID=XXX)
                 LDSET(PRESET=INDEF)
                 BINARY(PL=25000)
                 7/8/9 CARD
                                 .
                                 .
                                 .
                                 .
                 6/7/8/9 CARD
```

Fig. 3.6: Execution of the analysis by loading LASERFTN and KRFBIN, or the complete binary file KRFLASER.

```
Control Cards
SYNTH,TXXX,IOXXX,PX.
USER(ABC,XYZ)
PROJECT(*NNN*NAME)
ATTACH(OLDPL,LASERBCD,ID=XXX)
ATTACH(OBJ,LASERFTN,ID=XXX)
ATTACH(TAPE8,CROSSSECTIONS,ID=XXX)
REQUEST,TAPE9,*PF.
REQUEST,BIN,*PF.
REQUEST,BIN1,*PF.
REQUEST,TAPE4,*PF.
REQUEST,NEWPL,*PF.
UPDATE(P,L=1)
FTN(I=COMPILE,R=3,A,EL=F)
REWIND(OBJ,LGO)
COPYL(OBJ,LGO,BIN)
CATALOG(BIN,LASERFTN,ID=XXX)
PURGE(OBJ)
LDSET(PRESET=INDEF)
BIN.
UPDATE(N,I=TAPE3)
CATALOG(NEWPL,KRFBCD,ID=XXX)
FTN(I,B=BIN1,R=3,EL=F)
CATALOG(BIN1,KRFBIN,ID=XXX)
COPYL(BIN,BIN1,BINARY,,AR)
CATALOG(TAPE4,KRFDATA,ID=XXX)
LDSET(PRESET=INDEF)
BINARY(PL=25000)
CATALOG(TAPE9,CROSSSECTIONS,ID=XXX)
PURGE(TAPE8)
Update Program Library
7/8/9 CARD
     INSERTIONS AND DELETIONS
          .
          .
          .
7/8/9 CARD
DATA BLOCK 1
HEADER CARD
     ARBITRARILY LONG SEQUENCE OF REACTIONS
          .
          .
          .
DATA BLOCK 2
7/8/9 CARD
     STACKED E- CROSS SECTION PACKAGES
     (ARBITRARILY MANY ARE PERMITTED)
          .
          .
          .
DATA BLOCK 3
7/8/9 CARD
     COMMENT CARDS
          .
          .
          .
DATA BLOCK 4
7/8/9 CARD
     EXECUTION DATA PACKAGE
          .
          .
          .
7/8/9 CARD
6/7/8/9 CARD
```

Fig. 3.7: Synthesis and catalog of program KRFBCD under a modified version of LASERBCD, followed by execution of the analysis.

tain changes related to execution of the analysis (not involving the synthesis of subroutines), Fig. 3.8 contains the appropriate control card and input deck structure.

It is conceivable that the user may desire to make changes both in the main program LASER (or in any of its subroutines) and in the synthetic subroutines (JACOB, DNDT, or LEVELS). To facilitate this, it is convenient to have catalogued the BCD UPDATE program library KRFBCD (as described in Fig. 3.5). Both LASERBCD and KRFBCD can be updated, with their modified subroutines replaced (by COPYL) on the binary compilation file KRFLASER used for execution. It would be much more difficult to extend the translation capabilities of subroutine SYNTH to automatically recognize new reaction syntax, or to incorporate new computational features into the molecular kinetic subroutines, than it would be to merely modify the synthetic subroutines generated by the present program. There are, therefore, situations where an update of the program library KRFBCD (supplemented by any changes required for insuring compatibility with LASER or its subroutines) would probably be more efficient than an attempt to extend subroutine SYNTH. On the other hand, extensions which are likely to be of general applicability to future usage of the code should probably be incorporated directly into subroutine SYNTH.

Execution of the Boltzmann analysis program ELECT can be carried out with the control card sequence and data deck structure shown in Fig. 3.9. The electron cross section data library CROSSSECTIONS (discussed above) is compatible with either program (LASER, ELECT) and the structure of the electron update input (DATA BLOCK 2) is identical for both programs. Obviously, the same procedures for program modification by update of BOLTZBCD (as discussed for LASERBCD) are possible.

```
Control Cards
LASER,TXXX,IOXXX,PX.
USER(ABC,XYZ)
PROJECT(*NNN*NAME)
ATTACH(OLDPL,LASERBCD,ID=XXX)
ATTACH(OBJ,LASERFTN,ID=XXX)
ATTACH(TAPE8,CROSSSECTIONS,ID=XXX)
ATTACH(TAPE4,KRFDATA,ID=XXX)
ATTACH(BINARY,KRFBIN,ID=XXX)
REQUEST,TAPE9,*PF.
REQUEST,BIN,*PF.
UPDATE(P,L=1)
FTN(I=COMPILE,R=3,A,EL=F)
REDUCE.
REWIND(OBJ,LGO)
COPYL(OBJ,LGO,BIN)
CATALOG(BIN,LASERFTN,ID=XXX)
PURGE(OBJ)
LOAD(BINARY)
LDSET(PRESET=INDEF)
BIN(PL=25000)
CATALOG(TAPE9,CROSSSECTIONS,ID=XXX)
PURGE(TAPE8)
7/8/9 CARD
Update Program Library
*IDENT,-CHANGE-
     INSERTIONS AND DELETIONS
          .
          .
          .
7/8/9 CARD
DATA BLOCK 2
     STACKED E- CROSS SECTION PACKAGES
     (ARBITRARILY MANY PERMITTED)
          .
          .
          .
7/8/9 CARD
DATA BLOCK 3
     COMMENT CARDS
          .
          .
          .
7/8/9 CARD
 $CONTROL ... $
 $PARAM ... $
 $OPTICAL ... $
 $EBEAM ... $
 $CIRCUIT ... $
 $RATES ... $
DATA BLOCK 4
GAS1      P1        E1        M1
GAS2      P2        E2        M2
GAS3      P3        E3        M3
          .
          .
          .
GASK      PK        EK        MK
          .
          .
          .
7/8/9 CARD
6/7/8/9 CARD
```

Fig. 3.8: Program library LASERBCD is modified by update, previous binary file KRFBIN is loaded, and analysis is executed under new version of LASERFTN.

```
                BOLTZ,TXXX,IOXXX,PX.
Control         USER(ABC,XYZ)
Cards           PROJECT(*NNN*NAME)
                ATTACH(TAPE8,CROSSSECTIONS,ID=XXX)
                ATTACH(LGO,BOLTZFTN,ID=XXX)
                REDUCE.
                LDSET(PRESET=INDEF)
                LGO(PL=25000)
                7/8/9 CARD
                              .
                              .
                              .
DATA                          .
BLOCK 2              ELECTRON CROSS SECTION PACKAGES
                     (ARBITRARILY MANY ARE PERMITTED.)
                              .
                              .
                              .
                7/8/9 CARD
                AR + E ↱ AR* + E
                AR + E ↱ AR** + E
                AR + E ↱ AR(+) + E + E
                              .
                              .
DATA                          .
BLOCK A              SECONDARY ELECTRON COLLISION PROCESSES
                     INCLUDED IN THE BOLTZMANN ANALYSIS
                              .
                              .
                              .
                7/8/9 CARD
                 $CONTROL ... $
                 $PARAM ... $
DATA             $SOURCE ... $
BLOCK B1        GAS1      P1      E1      M1
                GAS2      P2      E2      M2
                GAS3      P3      E3      M3
                              .
                              .
                              .
                7/8/9 CARD
                 $CONTROL ... $
                 $PARAM ... $
DATA             $SOURCE ... $
BLOCK B2        GAS1      P1      E1      M1
                GAS2      P2      E2      M2
                              .
                              .
                              .
                7/8/9 CARD
                              .
      .                       .
      .                       .
      .                       .
                6/7/8/9 CARD
```

Fig. 3.9: Execution of the Boltzmann program ELECT.

4.0 KrF LASER KINETICS: Illustrative Example of Program Synthesis and Execution

The Computer Program LASER that was described in Sec. 3 can be used to (automatically) synthesize and execute (for a reasonably arbitrary reaction scheme) a coupled analysis of molecular kinetics, electron kinetics, radiative extraction, and external (RLC) driving circuit. In this section, usage of the code will be illustrated with sample output obtained from analysis of the KrF laser kinetic system[1-5]. Names of permanent files in the discussion of control cards in Sec. 3.5 were chosen in anticipation of this example.

4.1 Molecular Kinetic Subroutine Generation

As many as 80 reactions have been proposed as being of possible importance for the KrF laser kinetic reaction scheme. Fig. 4.1 shows the "playback" (generated in output by subroutine EDITOR) of the exact input card images of DATA BLOCK 1 (used in the deck structure of Fig. 3.5, for example) for synthesis of a KrF laser kinetics analysis. The header Card 1 contains three (10 BCD character) computer words (" NORTHROP ", "KRF LASER ", and "KINETICS ") which name the generated program and are used for a three-line block-letter title in subsequent output. Following the header card, there are 80 pairs of cards which define the kinetic reaction scheme and its rate constants (cf. description of DATA BLOCK 1 in Sec. 3.2).

The reactions of Fig. 4.1 are processed by Subroutine SYNTH and are translated into FORTRAN subroutines (JACOB, DNDT, and LEVELS). During the translation process, Subroutine SYNTH also generates its own COMMENT card documentation of the synthesized subroutines in

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
(DATE: 01/04/79)

```
CARD                1         2         3         4         5         6         7         8
 NO.     12345678901234567890123456789012345678901234567890123456789012345678901234567890
--------------------------------------------------------------------------------------------

  1 ...  NORTHROP KRF LASER KINETICS
  2 ...AR + E → AR* + E
  3 ...                                SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45
  4 ...KR + E → KR* + E
  5 ...                                SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45
  6 ...AR + E → AR** + E
  7 ...                                0.1 X AR* CROSS SECTION, 13.4 EV THRESH
  8 ...KR + E → KR** + E
  9 ...                                0.1 X AR* CROSS SECTION, 11.5 EV THRESH
 10 ...AR* + E → AR** + E
 11 ...                                60.E-16 CM2 AT 2 EV THRESHHOLD ASSUMED.
 12 ...KR* + E → KR** + E
 13 ...                                60.E-16 CM2 AT 1.6 EV THRESHHOLD ASSUMED.
 14 ...AR + E → AR(+) + E + E
 15 ...                                RAPP, ENGLANDER-GOLDEN JCP 43, 1464 (65)
 16 ...KR + E → KR(+) + E + E
 17 ...                                RAPP, ENGLANDER-GOLDEN JCP 43, 1464 (65)
 18 ...AR* + E → AR(+) + E + E
 19 ...                                7.E-16 CM2 AT 4.2 EV THRESHHOLD ASSUMED.
 20 ...KR* + E → KR(+) + E + E
 21 ...                                10.E-16 CM2 AT 4.0 EV THRESHHOLD ASSUMED.
 22 ...AR** + E → AR(+) + E + E
 23 ...                                30 E-16 CM2 AT 2.4 EV THRESHOLD.
 24 ...KR** + E → KR(+) + E + E
 25 ...                                30 E-16 CM2 AT 3.1 EV THRESHOLD.
 26 ...AR2(+) + E → AR* + AR
 27 ...                                MEHR, BIONDI (SYNTHETIC: TE**(-3/2) LAW)
 28 ...KR2(+) + E → KR* + KR
 29 ...                                OSKAM, MITTELSTADT (SYNTHETIC: TE**(-3/2) LAW)
 30 ...F2 + E → F + F-
 31 ...                                HOFLAND, AEROSPACE CORP.
 32 ...AR2* + E → AR + AR + E
 33 ...  1.00 E-07
 34 ...KR2* + E → KR + KR + E
 35 ...  1.00 E-07
 36 ...AR + HE- → AR(+) + HE- + E
 37 ...  4.34 E-18                    BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV)
 38 ...AR + HE- → AR* + HE-
 39 ...  1.24 E-18 1.24 E-18          (1/3.5) X AR + HE → AR(+) + E + HE
 40 ...KR + HE- → KR(+) + HE- + E
--------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme.

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
(DATE: 01/04/79)

```
CARD                1         2         3         4         5         6         7         8
 NO.     12345678901234567890123456789012345678901234567890123456789012345678901234567890
--------------------------------------------------------------------------------------------

 41 ...., 8.04 E-18                 BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV)
 42 ....KR + HE- → KR* + HE-
 43 ....,2.30 E-18 2.30 E-18        (1/3.5) X KR + HE → KR(+) + E + HE
 44 ....AR(+) + AR + M → AR2(+) + M
 45 ....,2.00 E-31                  W. F. LIU, D. C. CONWAY  JCP 62, 3070 (1975)
 46 ....AR(+) + KR + M → ARKR(+) + M
 47 ....,   2.5E-31
 48 ....KR(+) + KR + M →KR2(+) + M
 49 ....,2.40 E-31                  C. J. TRACY, H. J. OSKAM  JCP 65, 3387 (1976)
 50 ....KR(+) + AR + M → ARKR(+) + M
 51 ....,   1.0E-31
 52 ....AR(+) + KR → AR + KR(+)
 53 ....,3.00 E-11
 54 ....AR2(+) + KR → KR(+) + AR + AR
 55 ....,   7.5E-10                 BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
 56 ....ARKR(+) + KR → KR2(+) + AR
 57 ....,   3.2E-10                 BOHME ET AL, J. CHEM. PHYS. 52, 5094  (1970)
 58 ....AR* + AR + M → AR2* + M
 59 ....,1.00 E-32                  HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974.
 60 ....AR* + KR + M → ARKR* + M
 61 ....,   1.0E-32
 62 ....KR* + KR + M → KR2* + M
 63 ....,   5.5E-32                 HUGHES LASL ASPEN 9/76
 64 ....KR* + AR + M → ARKR* + M
 65 ....,   1.0E-32
 66 ....ARKR* + KR → KR2* + AR
 67 ....,1.00 E-10                  SRI REPORT NO. MP 76-99, DEC., 1976
 68 ....AR2(+) + F- → ARF* + AR
 69 ....,5.00 E-07
 70 ....AR2(+) + F- → AR2F*
 71 ....,5.00 E-07
 72 ....AR(+) + F- → ARF*
 73 ....,   1.0E-06
 74 ....KR2(+) + F- → KRF* + KR
 75 ....,5.00 E-07
 76 ....KR2(+) + F- → KR2F*
 77 ....,5.00 E-07
 78 ....KR(+) + F- → KRF*
 79 ....,   1.0E-06
 80 ....ARKR(+) + F- → KRF* + AR
--------------------------------------------------------------------------------------------

     12345678901234567890123456789012345678901234567890123456789012345678901234567890
                1         2         3         4         5         6         7         8
```

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme. (Continued)

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                              (DATE: 01/04/79)

CARD            1         2         3         4         5         6         7         8
 NO.    12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------------

 81 ...  5.00 E-07
 82 ...ARKR(+) + F- → ARKRF*
 83 ...  5.00 E-07
 84 ...KR* + F2 → KRF* + F
 85 ...  7.20 E-10                VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
 86 ...AR* + F2 → ARF* + F
 87 ...  7.50 E-10                VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
 88 ...AR* + KR → AR + KR*
 89 ...  6.20 E-12                PIPER, SETSER, CLYNE, JCP 63, 4018 (1975)
 90 ...KRF* + AR + M → ARKRF* + M
 91 ...  6.00 E-32                AVCO
 92 ...KRF* + KR + M → KR2F* + M
 93 ...  5.00 E-31                AVCO
 94 ...ARF* + AR + M → AR2F* + M
 95 ...  4.00 E-31                AVCO
 96 ...ARF* + KR + M → ARKRF* + M
 97 ...  1.00 E-31
 98 ...AR2* + KR → AR + AR + KR*
 99 ...  8.00 E-11                ZAMIR (PRIV. COMMUN. TO SRI)
100 ...AR2* + AR2* → AR2(+) + AR + AR + E
101 ...    3.0E-10
102 ...ARF* + KR → KRF* + AR
103 ...  1.50 E-10                SRI REPORT NO. MP 76-99, DEC., 1976
104 ...AR2* + F → ARF* + AR
105 ...    3.0E-10
106 ...KR2* + F → KRF* + KR
107 ...    3.0E-10
108 ...AR2* + F2 → AR2F* + F
109 ...  2.50 E-10                SRI REPORT NO. MP 76-99, DEC., 1976
110 ...ARKR* + F2 → KRF* + AR + F
111 ...  6.00 E-10                SRI REPORT NO. MP 76-99, DEC., 1976
112 ...ARKR* + F2 → ARKRF* + F
113 ...    3.0E-10
114 ...KR2* + F2 → KR2F* + F
115 ...  3.00 E-10                SRI REPORT NO. MP 76-99, DEC., 1976
116 ...AR2F* + F2 → AR + AR + F + F2
117 ...  1.00 E-09                SRI REPORT NO. MP 76-99, DEC., 1976
118 ...ARKRF* + F2 → AR + KR + F + F2
119 ...  1.00 E-09                SRI REPORT NO. MP 76-99, DEC., 1976
120 ...KR2F* + F2 → KR + KR + F + F2
-------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme. (Continued)

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                                (DATE: 01/04/79)

CARD          1         2         3         4         5         6         7         8
 NO.   12345678901234567890123456789012345678901234567890123456789012345678901234567890
-----------------------------------------------------------------------------------------

121 .... 1.00 E-09                SRI REPORT NO. MP 76-99, DEC., 1976
122 ....ARKRF* + KR → KR2F* + AR
123 .... 1.00 E-10                SRI REPORT NO. MP 76-99, DEC., 1976
124 ....KRF* + F2 → KR + F + F2
125 .... 1.00 E-09                SRI REPORT NO. MP 76-99, DEC., 1976
126 ....ARF* + F2 → AR + F + F2
127 .... 1.00 E-09                SRI REPORT NO. MP 76-99, DEC., 1976
128 ....AR2F* + KR → KRF* + AR + AR
129 ....   1.0E-10
130 ....AR** + M → AR* + M
131 .... 1.00 E-10
132 ....KR** + M → KR* + M
133 .... 1.00 E-10
134 ....ARF* → AR + F
135 .... 3.30 E 07                SRI REPORT NO. MP 76-99, DEC., 1976
136 ....AR2* → AR + AR
137 .... 3.80 E 06                SRI REPORT NO. MP 76-99, DEC., 1976
138 ....ARKR* → AR + KR
139 ....   3.0E+06
140 ....KR2* → KR + KR
141 .... 3.30 E 06                SRI REPORT NO. MP 76-99, DEC., 1976
142 ....AR2F* → AR + AR + F
143 .... 2.00 E 08                SRI REPORT NO. MP 76-99, DEC., 1976
144 ....ARKRF* → AR + KR + F
145 .... 5.00 E 07                SRI REPORT NO. MP 76-99, DEC., 1976
146 ....KR2F* → KR + KR + F
147 .... 6.70 E 07                SRI REPORT NO. MP 76-99, DEC., 1976
148 ....KRF* → KR + F + HNU
149 .... 1.10 E 08                R. BURNHAM, S. 5. SEARLES (SUBMITTED TO JCP)
150 ....KRF* + RAD → KR + F + RAD
151 .... 2.00 E-16                LASER TRANSITION: STIMULATED EMISSION X-SECTION
152 ....F2 + RAD → F + F
153 .... 1.50 E-20
154 ....F- + RAD → F + E
155 .... 5.40 E-18                A. MANDL, PHYS REV A3, 251 (1971)
156 ....KR2F* + RAD → AR* + KR + F
157 .... 1.00 E-99                CROSS SECTION UNKNOWN
158 ....AR2(+) + RAD → AR + AR(+)
159 .... 1.50 E-17                STEVENS (PARK CITY CONFERENCE)
160 ....KR2(+) + RAD → KR + KR(+)
-----------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme. (Continued)

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                                (DATE: 01/04/79)

CARD            1         2         3         4         5         6         7         8
 NO.   12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------------

161 .... 3.50 E-18                J. WEST (NRTC)
-------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                1         2         3         4         5         6         7         8
```

Fig. 4.1: DATA BLOCK 1 card input for definition of KrF kinetic reaction scheme. (Continued)

order to make them completely readable and accessible to modification. Fig. 4.2, 4.3, and 4.4 present samples of the FORTRAN statements generated for subroutines DNDT, JACOB, and LEVELS, respectively. Although it would be impractical to reproduce the entire listings of these synthesized subroutines here, it is informative to present excerpts which illustrate the translation for miscellaneous representative types of collisions, as is done in Fig. 4.2 and 4.3.

As the reaction queue of DATA BLOCK 1 is scanned by Subroutine SYNTH, input reference data, informative comments, and/or warning diagnostics are generated to produce an output summary, shown in Fig. 4.5. A reaction with unacceptable syntax or content is ignored, although processing continues. (An ignored reaction is not assigned a number in the summary of Fig. 4.5.) After the entire reaction list has been processed, a cross-reference table, illustrated by Fig. 4.6, is generated. This table provides for rapid identification of all reactions that involve any particular species, and is convenient whenever it is desired to delete some species from the kinetic scheme.

After generation of the FORTRAN source code on TAPE3 and construction of the data file on TAPE4, there is an exit from program LASER. TAPE3 is used as the source for creation of a BCD UPDATE file (cf. Fig. 3.5) which is catalogued as KRFBCD, and its binary compilation is combined with LASERFTN to create file KRFLASER for execution. The data file on TAPE4 is catalogued as KRFDATA.

4.2 Execution of the Analysis

With the use of permanent files KRFDATA and KRFLASER, the analysis can be executed, either as a continuation from the initial synthesis

```
      SUBROUTINE DNDT (N, T, NO, NDOT)
C
C  ..................................................................
C
C     THIS SUBROUTINE WAS SYNTHESIZED BY EDITING AN INPUT FILE OF SYM-
C     BOLIC REACTIONS WHICH DEFINE A COUPLED SYSTEM OF ELECTRON AND
C     MOLECULAR KINETICS. IT RETURNS THE RATES NDOT(I) = (D/DT)NO(I),
C     I = 1,2,...NTYPE (CM-3/SEC). RATE CONSTANTS KF AND KR HAVE UNITS
C     OF CM2, SEC-1, CM3/SEC, CM6/SEC, ... AS APPROPRIATE.
C
C     THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-
C     ERATED THIS SUBROUTINE WAS DEVELOPED BY --
C
C                 ------------------------------------
C                 I                                  I
C                 I   DR. WILLIAM B. LACINA          I
C                 I   NORTHROP RESEARCH AND TECHNOLOGY I
C                 I   ONE RESEARCH PARK              I
C                 I   PALOS VERDES PENINSULA, CA 90274 I
C                 I   TEL: (213) 377-4811, EXT. 322  I
C                 I                                  I
C                 ------------------------------------
C
C  ..................................................................
C
      DIMENSION NO(1), NDOT(1)
      REAL NO, NTOT, NDOT, NOISE, NE, KF, KR, KB, KT, MU, LO, IBEAM,
     1 JBEAM, LENGTH
C
      COMMON / DATA / RATE( 200), KF( 200), KR( 200), VSIG(2, 25), E(30)
      COMMON / CONST / NTOT, TMOL, FREQ, HNU
      COMMON / DISCH / LO, CO, RO, MU, AREA, D
      COMMON / SOURCE / UPLUS, JBEAM, DVDX, DEPOSIT, ENERGY, SB, SO
      COMMON / GAINS / ALPHA, GAMMA, GAIN, ABSORB, OMEGA, LENGTH, CAVITY
C
      DATA KB, EO, H, C, PI / 8.614E-05, 1.602E-19, 6.625E-34,
     1     3.000E+10, 3.14159 /
C
      IBEAM = JBEAM*DEPOSIT*SHAPE(T)
      KT = KB*TMOL
      DO 1 I = 1,N
    1 NDOT(I) = 0.
      NDOT(1) = - C*GAMMA*NO(1)
      ALPHA = GAIN = HNU = FREQ = NOISE = DVDX = 0.
      SB = SO = 0.0
C
C     GAIN   = SIGMA*(N2-N1) IS THE LASER TRANSITION GAIN
C     ABSORB = SUMK[SIGMA(K)*NK] IS THE TOTAL ABSORPTION OF THE MEDIUM
C     ALPHA  = (GAIN-ABSORB) IS THE NET GAIN IN THE MEDIUM
C     GAMMA  = THRESHHOLD GAIN COEFFICIENT (CM-1)
C
C     CAVITY = MIRROR SEPARATION (CM)
C     LENGTH = LENGTH OF ACTIVE MEDIUM (CM)
C     OMEGA  = AREA/CAVITY**2
C     AREA   = AREA OF OPTICS (CM2)
C     GAMMA  = [LOSS + LN(1/R)/2]/LENGTH
C
```

Fig. 4.2: (Synthesized) Subroutine DNDT listing.

```
C  ..................................................................  DNDT
C                                                                      DNDT
C  THE FOLLOWING REACTIONS DEFINE THE KINETICS --                      DNDT
C                                                                      DNDT
C  1  AR + E → AR* + E                                                 DNDT
C                                                                      DNDT
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KF(  1) = VSIG(1, 1)                                         DNDT
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KR(  1) = VSIG(2, 1)                                         DNDT
C                                                                      DNDT
      R = KF(1)*NO(3)*NO(2) - KR(1)*NO(4)*NO(2)                        DNDT
C                                                                      DNDT
          RATE(  1) = R                                                DNDT
          NDOT(3) = NDOT(3) - R                                        DNDT
          NDOT(4) = NDOT(4) + R                                        DNDT
C                                                                      DNDT
C  2  KR + E → KR* + E                                                 DNDT
C                                                                      DNDT
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KF(  2) = VSIG(1, 2)                                         DNDT
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KR(  2) = VSIG(2, 2)                                         DNDT
C                                                                      DNDT
      R = KF(2)*NO(5)*NO(2) - KR(2)*NO(6)*NO(2)                        DNDT
C                                                                      DNDT
          RATE(  2) = R                                                DNDT
          NDOT(5) = NDOT(5) - R                                        DNDT
          NDOT(6) = NDOT(6) + R                                        DNDT
C                                                                      DNDT
C  3  AR + E → AR** + E                                                DNDT
C                                                                      DNDT
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KF(  3) = VSIG(1, 3)                                         DNDT
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KR(  3) = VSIG(2, 3)                                         DNDT
C                                                                      DNDT
      R = KF(3)*NO(3)*NO(2) - KR(3)*NO(7)*NO(2)                        DNDT
C                                                                      DNDT
          RATE(  3) = R                                                DNDT
          NDOT(3) = NDOT(3) - R                                        DNDT
          NDOT(7) = NDOT(7) + R                                        DNDT
C                                                                      DNDT
C  4  KR + E → KR** + E                                                DNDT
C                                                                      DNDT
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KF(  4) = VSIG(1, 4)                                         DNDT
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS             DNDT
          KR(  4) = VSIG(2, 4)                                         DNDT
C                                                                      DNDT
      R = KF(4)*NO(5)*NO(2) - KR(4)*NO(8)*NO(2)                        DNDT
C                                                                      DNDT
          RATE(  4) = R                                                DNDT
          NDOT(5) = NDOT(5) - R                                        DNDT
          NDOT(8) = NDOT(8) + R                                        DNDT
C                                                                      DNDT
C  5  AR* + E → AR** + E                                               DNDT
```

Fig. 4.2 (Continued)

```
C                                                                       DNDT    140
C  7  AR + E → AR(+) + E + E                                            DNDT    141
C                                                                       DNDT    142
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS              DNDT    143
          KF(  7) = VSIG(1, 7)                                          DNDT    144
C                                                                       DNDT    145
      R = KF(7)*NO(3)*NO(2)                                             DNDT    146
C                                                                       DNDT    147
          RATE(  7) = R                                                 DNDT    148
          NDOT(2) = NDOT(2) + R                                         DNDT    149
          NDOT(3) = NDOT(3) - R                                         DNDT    150
          NDOT(9) = NDOT(9) + R                                         DNDT    151
C                                                                       DNDT    152


C                                                                       DNDT    212
C 13  AR2(+) + E → AR* + AR                                             DNDT    213
C                                                                       DNDT    214
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS              DNDT    215
          KF( 13) = VSIG(1,13)                                          DNDT    216
C                                                                       DNDT    217
      R = KF(13)*NO(11)*NO(2)                                           DNDT    218
C                                                                       DNDT    219
          RATE( 13) = R                                                 DNDT    220
          NDOT(2) = NDOT(2) - R                                         DNDT    221
          NDOT(3) = NDOT(3) + R                                         DNDT    222
          NDOT(4) = NDOT(4) + R                                         DNDT    223
          NDOT(11) = NDOT(11) - R                                       DNDT    224
C                                                                       DNDT    225


C                                                                       DNDT    251
C 16  AR2* + E → AR + AR + E                                            DNDT    252
C                                                                       DNDT    253
      R = KF(16)*NO(16)*NO(2)                                           DNDT    254
C                                                                       DNDT    255
          RATE( 16) = R                                                 DNDT    256
          NDOT(3) = NDOT(3) + R + R                                     DNDT    257
          NDOT(16) = NDOT(16) - R                                       DNDT    258
C                                                                       DNDT    259


C                                                                       DNDT    288
C 19  AR + HE- → AR* + HE-                                              DNDT    289
C                                                                       DNDT    290
      E1 = + E( 3)                                                      DNDT    291
      E2 = + E( 4)                                                      DNDT    292
      R = KF(19)*NO(3) - KR(19)*NO(4)                                   DNDT    293
      S = R                                                             DNDT    294
      R = R*IBEAM/E0                                                    DNDT    295
C                                                                       DNDT    296
          RATE( 19) = R                                                 DNDT    297
          NDOT(3) = NDOT(3) - R                                         DNDT    298
          NDOT(4) = NDOT(4) + R                                         DNDT    299
          U = (E2 - E1)                                                 DNDT    300
C                                                                       DNDT    301
C     E-BEAM ENERGY DEPOSITION --                                       DNDT    302
          DVDX = DVDX + U*S                                             DNDT    303
C                                                                       DNDT    304
```

Fig. 4.2 (Continued)

```
C 20  KR + HE- → KR(+) + HE- + E                                    DNDT    305
C                                                                   DNDT    306
      E1 = + E( 5)                                                  DNDT    307
      E2 = + E(10) + E( 2)                                          DNDT    308
      R = KF(20)*NO(5)                                              DNDT    309
      S = R                                                         DNDT    310
      R = R*IBEAM/EO                                                DNDT    311
C                                                                   DNDT    312
            RATE( 20) = R                                           DNDT    313
            NDOT(2) = NDOT(2) + R                                   DNDT    314
            NDOT(5) = NDOT(5) - R                                   DNDT    315
            NDOT(10) = NDOT(10) + R                                 DNDT    316
            U = (E2 - E1)                                           DNDT    317
C                                                                   DNDT    318
C     SECONDARY ELECTRON CREATION--                                 DNDT    319
            SB = SB + R                                             DNDT    320
            U = U + UPLUS                                           DNDT    321
C                                                                   DNDT    322
C     E-BEAM ENERGY DEPOSITION --                                   DNDT    323
            DVDX = DVDX + U*S                                       DNDT    324
C                                                                   DNDT    325


C                                                                   DNDT    359
C 24  KR(+) + KR + M → KR2(+) + M                                   DNDT    360
C                                                                   DNDT    361
      R = KF(24)*NO(10)*NO(5)*NTOT                                  DNDT    362
C                                                                   DNDT    363
            RATE( 24) = R                                           DNDT    364
            NDOT(5) = NDOT(5) - R                                   DNDT    365
            NDOT(10) = NDOT(10) - R                                 DNDT    366
            NDOT(12) = NDOT(12) + R                                 DNDT    367
C                                                                   DNDT    368


C                                                                   DNDT    377
C 26  AR(+) + KR → AR + KR(+)                                       DNDT    378
C                                                                   DNDT    379
C     REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --               DNDT    380
C                                                                   DNDT    381
      E1 = + E( 9) + E( 5)                                          DNDT    382
      E2 = + E( 3) + E(10)                                          DNDT    383
      KR( 26) = KF( 26)*EXP(-(E1-E2)/KT)                            DNDT    384
C                                                                   DNDT    385
      R = KF(26)*NO(9)*NO(5) - KR(26)*NO(3)*NO(10)                  DNDT    386
C                                                                   DNDT    387
            RATE( 26) = R                                           DNDT    388
            NDOT(3) = NDOT(3) + R                                   DNDT    389
            NDOT(5) = NDOT(5) - R                                   DNDT    390
            NDOT(9) = NDOT(9) - R                                   DNDT    391
            NDOT(10) = NDOT(10) + R                                 DNDT    392
C                                                                   DNDT    393


C                                                                   DNDT    658
C 50  AR2* + AR2* → AR2(+) + AR + AR + E                            DNDT    659
C                                                                   DNDT    660
      R = KF(50)*NO(16)*NO(16)                                      DNDT    661
C                                                                   DNDT    662
            RATE( 50) = R                                           DNDT    663
            NDOT(2) = NDOT(2) + R                                   DNDT    664
            NDOT(3) = NDOT(3) + R + R                               DNDT    665
            NDOT(11) = NDOT(11) + R                                 DNDT    666
            NDOT(16) = NDOT(16) - R - R                             DNDT    667
C                                                                   DNDT    668
C     CREATION OF (ZERO ENERGY) SECONDARY ELECTRONS--               DNDT    669
C                                                                   DNDT    670
            SO = SO + R                                             DNDT    671
C                                                                   DNDT    672
```

Fig. 4.2 (Continued)

```
C                                                                       DNDT    865
C 66  KR*+ + M → KR* + M                                                DNDT    866
C                                                                       DNDT    867
C     REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --                   DNDT    868
C                                                                       DNDT    869
      E1 = + E( 8)                                                      DNDT    870
      E2 = + E( 6)                                                      DNDT    871
      KR( 66) = KF( 66)*EXP(-(E1-E2)/KT)                                DNDT    872
C                                                                       DNDT    873
      R = KF(66)*NO(8)*NTOT - KR(66)*NO(6)*NTOT                         DNDT    874
C                                                                       DNDT    875
            RATE( 66) = R                                               DNDT    876
            NDOT(6) = NDOT(6) + R                                       DNDT    877
            NDOT(8) = NDOT(8) - R                                       DNDT    878


C                                                                       DNDT    879
C 67  ARF+ → AR + F                                                     DNDT    880
C                                                                       DNDT    881
      R = KF(67)*NO(20)                                                 DNDT    882
C                                                                       DNDT    883
            RATE( 67) = R                                               DNDT    884
            NDOT(3) = NDOT(3) + R                                       DNDT    885
            NDOT(14) = NDOT(14) + R                                     DNDT    886
            NDOT(20) = NDOT(20) - R                                     DNDT    887
C                                                                       DNDT    888


C                                                                       DNDT    941
C 74  KRF+ → KR + F + HNU                                               DNDT    942
C                                                                       DNDT    943
      R = KF(74)*NO(22)                                                 DNDT    944
C                                                                       DNDT    945
            RATE( 74) = R                                               DNDT    946
            NDOT(5) = NDOT(5) + R                                       DNDT    947
            NDOT(14) = NDOT(14) + R                                     DNDT    948
            NDOT(22) = NDOT(22) - R                                     DNDT    949
C                                                                       DNDT    950
C     PHOTON NUMBER DENSITY INCREASED BY NOISE --                       DNDT    951
C                                                                       DNDT    952
            NOISE = NOISE + R*OMEGA/4./PI                               DNDT    953
C                                                                       DNDT    954


C 75  KRF+ + RAD → KR + F + RAD                                         DNDT    955
C                                                                       DNDT    956
C     (STIMULATED EMISSION PROCESS, WITH NO( 1) = INTEN/C/HNU)          DNDT    957
C                                                                       DNDT    958
      E1 = + E(22) + E( 1)                                              DNDT    959
      E2 = + E( 5) + E(14) + E( 1)                                      DNDT    960
      HNU = E0*(E1 - E2)                                                DNDT    961
      FREQ = HNU/H                                                      DNDT    962
C                                                                       DNDT    963
      R = KF(75)*NO(22)*NO(1)                                           DNDT    964
      R = R*C                                                           DNDT    965
C                                                                       DNDT    966
            RATE( 75) = R                                               DNDT    967
            NDOT(1) = NDOT(1) + R                                       DNDT    968
            NDOT(5) = NDOT(5) + R                                       DNDT    969
            NDOT(14) = NDOT(14) + R                                     DNDT    970
```

Fig. 4.2 (Continued)

```
            NDOT(22) = NDOT(22) - R
C
      R = KF(75)*NO(22)
            GAIN = GAIN + R
            ALPHA = ALPHA + R
C
C 76  F2 + RAD ↱ F + F
C
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(76)*NO(13)*NO(1)
      R = R*C
C
            RATE( 76) = R
            NDOT(1) = NDOT(1) - R
            NDOT(13) = NDOT(13) - R
            NDOT(14) = NDOT(14) + R + R
C
      R = KF(76)*NO(13)
            ALPHA = ALPHA - R
C
C 77  F- + RAD ↱ F + E
C
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(77)*NO(15)*NO(1)
      R = R*C
C
            RATE( 77) = R
            NDOT(1) = NDOT(1) - R
            NDOT(2) = NDOT(2) + R
            NDOT(14) = NDOT(14) + R
            NDOT(15) = NDOT(15) - R
C
C     CREATION OF (ZERO ENERGY) SECONDARY ELECTRONS--
C
            S0 = S0 + R
C
      R = KF(77)*NO(15)
            ALPHA = ALPHA - R
C
C 78  KR2F* + RAD ↱ AR* + KR + F
C
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(78)*NO(23)*NO(1)
      R = R*C
C
            RATE( 78) = R
            NDOT(1) = NDOT(1) - R
            NDOT(4) = NDOT(4) + R
            NDOT(5) = NDOT(5) + R
            NDOT(14) = NDOT(14) + R
            NDOT(23) = NDOT(23) - R
C
      R = KF(78)*NO(23)
            ALPHA = ALPHA - R
```

Fig. 4.2 (Continued)

```
C                                                                       DNDT    1028
C 79  AR2(+) + RAD → AR + AR(+)                                         DNDT    1029
C                                                                       DNDT    1030
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)         DNDT    1031
C                                                                       DNDT    1032
      R = KF(79)*NO(11)*NO(1)                                           DNDT    1033
      R = R*C                                                           DNDT    1034
C                                                                       DNDT    1035
            RATE( 79) = R                                               DNDT    1036
            NDOT(1) = NDOT(1) - R                                       DNDT    1037
            NDOT(3) = NDOT(3) + R                                       DNDT    1038
            NDOT(9) = NDOT(9) + R                                       DNDT    1039
            NDOT(11) = NDOT(11) - R                                     DNDT    1040
C                                                                       DNDT    1041
      R = KF(79)*NO(11)                                                 DNDT    1042
            ALPHA = ALPHA - R                                           DNDT    1043
C                                                                       DNDT    1044
C 80  KR2(+) + RAD → KR + KR(+)                                         DNDT    1045
C                                                                       DNDT    1046
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)         DNDT    1047
C                                                                       DNDT    1048
      R = KF(80)*NO(12)*NO(1)                                           DNDT    1049
      R = R*C                                                           DNDT    1050
C                                                                       DNDT    1051
            RATE( 80) = R                                               DNDT    1052
            NDOT(1) = NDOT(1) - R                                       DNDT    1053
            NDOT(5) = NDOT(5) + R                                       DNDT    1054
            NDOT(10) = NDOT(10) + R                                     DNDT    1055
            NDOT(12) = NDOT(12) - R                                     DNDT    1056
C                                                                       DNDT    1057
      R = KF(80)*NO(12)                                                 DNDT    1058
            ALPHA = ALPHA - R                                           DNDT    1059
C                                                                       DNDT    1060
C     COMPUTE FINAL EXPRESSION FOR D/DT(PHOTON DENSITY) --              DNDT    1061
C                                                                       DNDT    1062
      NDOT(1) = (LENGTH/CAVITY)*(NDOT(1) + NOISE)                       DNDT    1063
C                                                                       DNDT    1064
      ABSORB = GAIN - ALPHA                                             DNDT    1065
      DVDX = DEPOSIT*DVDX                                               DNDT    1066
C                                                                       DNDT    1067
C  ..................................................................   DNDT    1068
C                                                                       DNDT    1069
C     EXTERNAL CIRCUIT EQUATIONS (Q → NO(25), AND I → NO(26)) --        DNDT    1070
C                                                                       DNDT    1071
      NE = NO(2)                                                        DNDT    1072
      IF (NE.EQ.0.) NE = 1.0                                            DNDT    1073
      CONDUCT = NE*E0*MU                                                DNDT    1074
      RD = D/AREA/CONDUCT                                               DNDT    1075
C                                                                       DNDT    1076
      IF (L0.EQ.0.) GO TO 2                                             DNDT    1077
      DQDT = NDOT(25) = NO(26)                                          DNDT    1078
      DIDT = NDOT(26) = (-NO(25)/C0 - (R0 + RD)*NO(26))/L0              DNDT    1079
      RETURN                                                            DNDT    1080
C                                                                       DNDT    1081
    2 DQDT = NDOT(25) = - NO(25)/C0/(R0 + RD)                           DNDT    1082
      CURRENT = NO(26) = NDOT(25)                                       DNDT    1083
C                                                                       DNDT    1084
C  ..................................................................   DNDT    1085
C                                                                       DNDT    1086
C  THE FOLLOWING MOLECULAR SPECIES (WITH LABELS) WERE INCLUDED --       DNDT    1087
C                                                                       DNDT    1088
C   1   RAD        2   E(-)       3   AR        4   AR*                 DNDT    1089
C   5   KR         6   KR*        7   AR**      8   KR**                DNDT    1090
C   9   AR(+)      10  KR(+)      11  AR2(+)    12  KR2(+)              DNDT    1091
C  13   F2         14  F          15  F-        16  AR2*               DNDT    1092
C  17   KR2*       18  ARKR(+)    19  ARKR*     20  ARF*                DNDT    1093
C  21   AR2F*      22  KRF*       23  KR2F*     24  ARKRF*              DNDT    1094
C                                                                       DNDT    1095
C  ..................................................................   DNDT    1096
C                                                                       DNDT    1097
      RETURN                                                            DNDT    1098
      END                                                               DNDT    1099
```

Fig. 4.2 (Continued)

```
      SUBROUTINE JACOB (N, T, NO, PHI)
C
C  ..................................................................
C
C     THIS SUBROUTINE WAS SYNTHESIZED BY EDITING AN INPUT FILE OF SYM-
C     BOLIC REACTIONS WHICH DEFINE A COUPLED SYSTEM OF ELECTRON AND
C     MOLECULAR KINETICS EQUATIONS.  IT RETURNS THE JACOBIAN MATRIX,
C
C                    PHI(I,J) = D[NDOT(I)]/D[NO(J)]
C
C     WHERE I,J = 1,2,3,...NTYPE.  N IS THE DIMENSION DECLARATOR FOR PHI
C     IN THE CALLING PROGRAM.  THE RATE CONSTANTS KF AND KR HAVE UNITS
C     OF CM2, SEC-1, CM3/SEC, CM6/SEC, ... AS APPROPRIATE.
C
C     THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-
C     ERATED THIS SUBROUTINE WAS DEVELOPED BY --
C
C              -----------------------------------
C              I                                 I
C              I   DR. WILLIAM B. LACINA         I
C              I   NORTHROP RESEARCH AND TECHNOLOGY I
C              I   ONE RESEARCH PARK             I
C              I   PALOS VERDES PENINSULA, CA 90274 I
C              I   TEL: (213) 377-4811, EXT. 322 I
C              I                                 I
C              -----------------------------------
C
C  ..................................................................
C
      DIMENSION PHI(N,1), NO(1)
      REAL NO, NTOT, NDOT, NOISE, NE, KF, KR, KB, KT, MU, LO, IBEAM,
     1 JBEAM, LENGTH
C
      COMMON / DATA / RATE( 200), KF( 200), KR( 200), VSIG(2, 25), E(30)
      COMMON / CONST / NTOT, TMOL, FREQ, HNU
      COMMON / DISCH / LO, CO, RO, MU, AREA, D
      COMMON / SOURCE / UPLUS, JBEAM, DVDX, DEPOSIT, ENERGY, SB, SO
      COMMON / GAINS / ALPHA, GAMMA, GAIN, ABSORB, OMEGA, LENGTH, CAVITY
C
      DATA KB, EO, H, C, PI / 8.614E-05, 1.602E-19, 6.625E-34,
     1     3.000E+10, 3.14159 /
C
      IBEAM = JBEAM*DEPOSIT*SHAPE(T)
      KT = KB*TMOL
      DO 1 I = 1,N
      DO 1 J = 1,N
    1 PHI(I,J) = 0.
      PHI(1,1) = - C*GAMMA
C
C     CAVITY = MIRROR SEPARATION (CM)
C     LENGTH = LENGTH OF ACTIVE MEDIUM (CM)
C     OMEGA  = AREA/CAVITY**2
C     AREA   = AREA OF OPTICS (CM2)
C     GAMMA  = [LOSS + LN(1/R)/2]/LENGTH
C
C  ..................................................................
C
```

Fig. 4.3: (Synthesized) Subroutine JACOB.

```
C  THE FOLLOWING REACTIONS DEFINE THE KINETICS --
C
C  1  AR + E → AR* + E
C
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KF(  1) = VSIG(1, 1)
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KR(  1) = VSIG(2, 1)
C
      R = KF(1)*NO(3)-KR(1)*NO(4)
C
          PHI( 3, 2) = PHI( 3, 2) - R
          PHI( 4, 2) = PHI( 4, 2) + R
C
      R = KF(1)*NO(2)
C
          PHI( 3, 3) = PHI( 3, 3) - R
          PHI( 4, 3) = PHI( 4, 3) + R
C
      R = -KR(1)*NO(2)
C
          PHI( 3, 4) = PHI( 3, 4) - R
          PHI( 4, 4) = PHI( 4, 4) + R
C
C  2  KR + E → KR* + E
C
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KF(  2) = VSIG(1, 2)
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KR(  2) = VSIG(2, 2)
C
      R = KF(2)*NO(5)-KR(2)*NO(6)
C
          PHI( 5, 2) = PHI( 5, 2) - R
          PHI( 6, 2) = PHI( 6, 2) + R
C
      R = KF(2)*NO(2)
C
          PHI( 5, 5) = PHI( 5, 5) - R
          PHI( 6, 5) = PHI( 6, 5) + R
C
      R = -KR(2)*NO(2)
C
          PHI( 5, 6) = PHI( 5, 6) - R
          PHI( 6, 6) = PHI( 6, 6) + R
C
C  3  AR + E → AR** + E
C
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KF(  3) = VSIG(1, 3)
C     REVERSE RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS
          KR(  3) = VSIG(2, 3)
C
      R = KF(3)*NO(3)-KR(3)*NO(7)
C
          PHI( 3, 2) = PHI( 3, 2) - R
          PHI( 7, 2) = PHI( 7, 2) + R
```

Fig. 4.3: (Continued)

```
C                                                                       JACOB    192
C  7  AR + E → AR(+) + E + E                                            JACOB    193
C                                                                       JACOB    194
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS              JACOB    195
          KF(  7) = VSIG(1, 7)                                          JACOB    196
C                                                                       JACOB    197
      R = KF(7)*NO(3)                                                   JACOB    198
C                                                                       JACOB    199
          PHI( 2, 2) = PHI( 2, 2) + R                                   JACOB    200
          PHI( 3, 2) = PHI( 3, 2) - R                                   JACOB    201
          PHI( 9, 2) = PHI( 9, 2) + R                                   JACOB    202
C                                                                       JACOB    203
      R = KF(7)*NO(2)                                                   JACOB    204
C                                                                       JACOB    205
          PHI( 2, 3) = PHI( 2, 3) + R                                   JACOB    206
          PHI( 3, 3) = PHI( 3, 3) - R                                   JACOB    207
          PHI( 9, 3) = PHI( 9, 3) + R                                   JACOB    208
C                                                                       JACOB    209
```

```
C                                                                       JACOB    294
C 13  AR2(+) + E → AR* + AR                                             JACOB    295
C                                                                       JACOB    296
C     FORWARD RATE IS OBTAINED FROM E(-) KINETICS ANALYSIS              JACOB    297
          KF( 13) = VSIG(1,13)                                          JACOB    298
C                                                                       JACOB    299
      R = KF(13)*NO(11)                                                 JACOB    300
C                                                                       JACOB    301
          PHI( 2, 2) = PHI( 2, 2) - R                                   JACOB    302
          PHI( 3, 2) = PHI( 3, 2) + R                                   JACOB    303
          PHI( 4, 2) = PHI( 4, 2) + R                                   JACOB    304
          PHI(11, 2) = PHI(11, 2) - R                                   JACOB    305
C                                                                       JACOB    306
      R = KF(13)*NO(2)                                                  JACOB    307
C                                                                       JACOB    308
          PHI( 2,11) = PHI( 2,11) - R                                   JACOB    309
          PHI( 3,11) = PHI( 3,11) + R                                   JACOB    310
          PHI( 4,11) = PHI( 4,11) + R                                   JACOB    311
          PHI(11,11) = PHI(11,11) - R                                   JACOB    312
C                                                                       JACOB    313
```

```
C                                                                       JACOB    351
C 16  AR2* + E → AR + AR + E                                            JACOB    352
C                                                                       JACOB    353
      R = KF(16)*NO(16)                                                 JACOB    354
C                                                                       JACOB    355
          PHI( 3, 2) = PHI( 3, 2) + R + R                               JACOB    356
          PHI(16, 2) = PHI(16, 2) - R                                   JACOB    357
C                                                                       JACOB    358
      R = KF(16)*NO(2)                                                  JACOB    359
C                                                                       JACOB    360
          PHI( 3,16) = PHI( 3,16) + R + R                               JACOB    361
          PHI(16,16) = PHI(16,16) - R                                   JACOB    362
C                                                                       JACOB    363
```

Fig. 4.3: (Continued)

```
C                                                                       JACOB    383
C 19  AR + HE- → AR* + HE-                                              JACOB    384
C                                                                       JACOB    385
      R = KF(19)*IBEAM/E0                                               JACOB    386
C                                                                       JACOB    387
            PHI( 3, 3) = PHI( 3, 3) - R                                 JACOB    388
            PHI( 4, 3) = PHI( 4, 3) + R                                 JACOB    389
C                                                                       JACOB    390
      R = -KR(19)*IBEAM/E0                                              JACOB    391
C                                                                       JACOB    392
            PHI( 3, 4) = PHI( 3, 4) - R                                 JACOB    393
            PHI( 4, 4) = PHI( 4, 4) + R                                 JACOB    394
C                                                                       JACOB    395
C 20  KR + HE- → KR(+) + HE- + E                                        JACOB    396
C                                                                       JACOB    397
      R = KF(20)*IBEAM/E0                                               JACOB    398
C                                                                       JACOB    399
            PHI( 2, 5) = PHI( 2, 5) + R                                 JACOB    400
            PHI( 5, 5) = PHI( 5, 5) - R                                 JACOB    401
            PHI(10, 5) = PHI(10, 5) + R                                 JACOB    402
C                                                                       JACOB    403


C                                                                       JACOB    443
C 24  KR(+) + KR + M → KR2(+) + M                                       JACOB    444
C                                                                       JACOB    445
      R = KF(24)*NO(10)*NTOT                                            JACOB    446
C                                                                       JACOB    447
            PHI( 5, 5) = PHI( 5, 5) - R                                 JACOB    448
            PHI(10, 5) = PHI(10, 5) - R                                 JACOB    449
            PHI(12, 5) = PHI(12, 5) + R                                 JACOB    450
C                                                                       JACOB    451
      R = KF(24)*NO(5)*NTOT                                             JACOB    452
C                                                                       JACOB    453
            PHI( 5,10) = PHI( 5,10) - R                                 JACOB    454
            PHI(10,10) = PHI(10,10) - R                                 JACOB    455
            PHI(12,10) = PHI(12,10) + R                                 JACOB    456
C                                                                       JACOB    457


C                                                                       JACOB    471
C 26  AR(+) + KR → AR + KR(+)                                           JACOB    472
C                                                                       JACOB    473
C     REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --                   JACOB    474
C                                                                       JACOB    475
      E1 = + E( 9) + E( 5)                                              JACOB    476
      E2 = + E( 3) + E(10)                                              JACOB    477
      KR( 26) = KF( 26)*EXP(-(E1-E2)/KT)                                JACOB    478
C                                                                       JACOB    479
      R = -KR(26)*NO(10)                                                JACOB    480
C                                                                       JACOB    481
            PHI( 3, 3) = PHI( 3, 3) + R                                 JACOB    482
            PHI( 5, 3) = PHI( 5, 3) - R                                 JACOB    483
            PHI( 9, 3) = PHI( 9, 3) - R                                 JACOB    484
            PHI(10, 3) = PHI(10, 3) + R                                 JACOB    485
C                                                                       JACOB    486
      R = KF(26)*NO(9)                                                  JACOB    487
C                                                                       JACOB    488
            PHI( 3, 5) = PHI( 3, 5) + R                                 JACOB    489
            PHI( 5, 5) = PHI( 5, 5) - R                                 JACOB    490
            PHI( 9, 5) = PHI( 9, 5) - R                                 JACOB    491
            PHI(10, 5) = PHI(10, 5) + R                                 JACOB    492
C                                                                       JACOB    493
```

Fig. 4.3 (Continued)

```
      R = KF(26)*NO(5)                                                  JACOB    494
C                                                                       JACOB    495
            PHI( 3, 9) = PHI( 3, 9) + R                                 JACOB    496
            PHI( 5, 9) = PHI( 5, 9) - R                                 JACOB    497
            PHI( 9, 9) = PHI( 9, 9) - R                                 JACOB    498
            PHI(10, 9) = PHI(10, 9) + R                                 JACOB    499
C                                                                       JACOB    500
      R = -KR(26)*NO(3)                                                 JACOB    501
C                                                                       JACOB    502
            PHI( 3,10) = PHI( 3,10) + R                                 JACOB    503
            PHI( 5,10) = PHI( 5,10) - R                                 JACOB    504
            PHI( 9,10) = PHI( 9,10) - R                                 JACOB    505
            PHI(10,10) = PHI(10,10) + R                                 JACOB    506
C                                                                       JACOB    507


C                                                                       JACOB   1009
C 50  AR2* + AR2* → AR2(+) + AR + AR + E                                JACOB   1010
C                                                                       JACOB   1011
      R = 2.*KF(50)*NO(16)                                              JACOB   1012
C                                                                       JACOB   1013
            PHI( 2,16) = PHI( 2,16) + R                                 JACOB   1014
            PHI( 3,16) = PHI( 3,16) + R + R                             JACOB   1015
            PHI(11,16) = PHI(11,16) + R                                 JACOB   1016
            PHI(16,16) = PHI(16,16) - R - R                             JACOB   1017
C                                                                       JACOB   1018


C 66  KR** + M → KR* + M                                                JACOB   1395
C                                                                       JACOB   1396
C     REVERSE RATE IS OBTAINED FROM DETAIL BALANCE --                   JACOB   1397
C                                                                       JACOB   1398
      E1 = + E( 8)                                                      JACOB   1399
      E2 = + E( 6)                                                      JACOB   1400
      KR( 66) = KF( 66)*EXP(-(E1-E2)/KT)                                JACOB   1401
C                                                                       JACOB   1402
      R = -KR(66)*NTOT                                                  JACOB   1403
C                                                                       JACOB   1404
            PHI( 6, 6) = PHI( 6, 6) + R                                 JACOB   1405
            PHI( 8, 6) = PHI( 8, 6) - R                                 JACOB   1406
C                                                                       JACOB   1407
      R = KF(66)*NTOT                                                   JACOB   1408
C                                                                       JACOB   1409
            PHI( 6, 8) = PHI( 6, 8) + R                                 JACOB   1410
            PHI( 8, 8) = PHI( 8, 8) - R                                 JACOB   1411
C                                                                       JACOB   1412
C 67  ARF* → AR + F                                                     JACOB   1413
C                                                                       JACOB   1414
      R = KF(67)                                                        JACOB   1415
C                                                                       JACOB   1416
            PHI( 3,20) = PHI( 3,20) + R                                 JACOB   1417
            PHI(14,20) = PHI(14,20) + R                                 JACOB   1418
            PHI(20,20) = PHI(20,20) - R                                 JACOB   1419
C                                                                       JACOB   1420


C                                                                       JACOB   1467
C 74  KRF* → KR + F + HNU                                               JACOB   1468
C                                                                       JACOB   1469
      R = KF(74)                                                        JACOB   1470
C                                                                       JACOB   1471
            PHI( 5,22) = PHI( 5,22) + R                                 JACOB   1472
            PHI(14,22) = PHI(14,22) + R                                 JACOB   1473
            PHI(22,22) = PHI(22,22) - R                                 JACOB   1474
C                                                                       JACOB   1475
C     PHOTON NUMBER DENSITY INCREASED BY NOISE --                       JACOB   1476
C                                                                       JACOB   1477
            R = R*OMEGA/4./PI                                           JACOB   1478
            PHI(1,22) = PHI(1,22) + R                                   JACOB   1479
```

Fig. 4.3 (Continued)

```
C                                                                       JACOB    1480
C 75  KRF* + RAD → KR + F + RAD                                         JACOB    1481
C                                                                       JACOB    1482
C     (STIMULATED EMISSION PROCESS, WITH NO( 1) = INTEN/C/HNU)          JACOB    1483
C                                                                       JACOB    1484
      R = KF(75)*NO(22)                                                 JACOB    1485
      R = R*C                                                           JACOB    1486
C                                                                       JACOB    1487
           PHI( 1, 1) = PHI( 1, 1) + R                                  JACOB    1488
           PHI( 5, 1) = PHI( 5, 1) + R                                  JACOB    1489
           PHI(14, 1) = PHI(14, 1) + R                                  JACOB    1490
           PHI(22, 1) = PHI(22, 1) - R                                  JACOB    1491
C                                                                       JACOB    1492
      R = KF(75)*NO(1)                                                  JACOB    1493
      R = R*C                                                           JACOB    1494
C                                                                       JACOB    1495
           PHI( 1,22) = PHI( 1,22) + R                                  JACOB    1496
           PHI( 5,22) = PHI( 5,22) + R                                  JACOB    1497
           PHI(14,22) = PHI(14,22) + R                                  JACOB    1498
           PHI(22,22) = PHI(22,22) - R                                  JACOB    1499
C                                                                       JACOB    1500


C 76  F2 + RAD → F + F                                                  JACOB    1501
C                                                                       JACOB    1502
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)         JACOB    1503
C                                                                       JACOB    1504
      R = KF(76)*NO(13)                                                 JACOB    1505
      R = R*C                                                           JACOB    1506
C                                                                       JACOB    1507
           PHI( 1, 1) = PHI( 1, 1) - R                                  JACOB    1508
           PHI(13, 1) = PHI(13, 1) - R                                  JACOB    1509
           PHI(14, 1) = PHI(14, 1) + R + R                              JACOB    1510
C                                                                       JACOB    1511
      R = KF(76)*NO(1)                                                  JACOB    1512
      R = R*C                                                           JACOB    1513
C                                                                       JACOB    1514
           PHI( 1,13) = PHI( 1,13) - R                                  JACOB    1515
           PHI(13,13) = PHI(13,13) - R                                  JACOB    1516
           PHI(14,13) = PHI(14,13) + R + R                              JACOB    1517
C                                                                       JACOB    1518
C 77  F- + RAD → F + E                                                  JACOB    1519
C                                                                       JACOB    1520
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)         JACOB    1521
C                                                                       JACOB    1522
      R = KF(77)*NO(15)                                                 JACOB    1523
      R = R*C                                                           JACOB    1524
C                                                                       JACOB    1525
           PHI( 1, 1) = PHI( 1, 1) - R                                  JACOB    1526
           PHI( 2, 1) = PHI( 2, 1) + R                                  JACOB    1527
           PHI(14, 1) = PHI(14, 1) + R                                  JACOB    1528
           PHI(15, 1) = PHI(15, 1) - R                                  JACOB    1529
C                                                                       JACOB    1530
      R = KF(77)*NO(1)                                                  JACOB    1531
      R = R*C                                                           JACOB    1532
C                                                                       JACOB    1533
           PHI( 1,15) = PHI( 1,15) - R                                  JACOB    1534
           PHI( 2,15) = PHI( 2,15) + R                                  JACOB    1535
           PHI(14,15) = PHI(14,15) + R                                  JACOB    1536
           PHI(15,15) = PHI(15,15) - R                                  JACOB    1537
C                                                                       JACOB    1538
C 78  KR2F* + RAD → AR* + KR + F                                        JACOB    1539
C                                                                       JACOB    1540
```

Fig. 4.3 (Continued)

```
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(78)*NO(23)
      R = R*C
C
           PHI( 1, 1) = PHI( 1, 1) - R
           PHI( 4, 1) = PHI( 4, 1) + R
           PHI( 5, 1) = PHI( 5, 1) + R
           PHI(14, 1) = PHI(14, 1) + R
           PHI(23, 1) = PHI(23, 1) - R
C
      R = KF(78)*NO(1)
      R = R*C
C
           PHI( 1,23) = PHI( 1,23) - R
           PHI( 4,23) = PHI( 4,23) + R
           PHI( 5,23) = PHI( 5,23) + R
           PHI(14,23) = PHI(14,23) + R
           PHI(23,23) = PHI(23,23) - R
C
C 79  AR2(+) + RAD → AR + AR(+)
C
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(79)*NO(11)
      R = R*C
C
           PHI( 1, 1) = PHI( 1, 1) - R
           PHI( 3, 1) = PHI( 3, 1) + R
           PHI( 9, 1) = PHI( 9, 1) + R
           PHI(11, 1) = PHI(11, 1) - R
C
      R = KF(79)*NO(1)
      R = R*C
C
           PHI( 1,11) = PHI( 1,11) - R
           PHI( 3,11) = PHI( 3,11) + R
           PHI( 9,11) = PHI( 9,11) + R
           PHI(11,11) = PHI(11,11) - R
C
C 80  KR2(+) + RAD → KR + KR(+)
C
C     (RADIATIVE ABSORPTION PROCESS, WITH NO( 1) = INTEN/C/HNU)
C
      R = KF(80)*NO(12)
      R = R*C
C
           PHI( 1, 1) = PHI( 1, 1) - R
           PHI( 5, 1) = PHI( 5, 1) + R
           PHI(10, 1) = PHI(10, 1) + R
           PHI(12, 1) = PHI(12, 1) - R
C
      R = KF(80)*NO(1)
      R = R*C
C
           PHI( 1,12) = PHI( 1,12) - R
           PHI( 5,12) = PHI( 5,12) + R
```

Fig. 4.3 (Continued)

```
      PHI(10,12) = PHI(10,12) + R                                       JACOB   1598
      PHI(12,12) = PHI(12,12) - R                                       JACOB   1599
C                                                                       JACOB   1600
      RATIO = LENGTH/CAVITY                                             JACOB   1601
      DO 3 I = 1,N                                                      JACOB   1602
    3 PHI(1,I) = RATIO*PHI(1,I)                                         JACOB   1603
C                                                                       JACOB   1604
C ..................................................................... JACOB   1605
C                                                                       JACOB   1606
C     EXTERNAL CIRCUIT EQUATIONS (Q = NO(25), AND I = NO(26)) --        JACOB   1607
C                                                                       JACOB   1608
      NE = NO(2)                                                        JACOB   1609
      IF (NE.EQ.0.) NE = 1.0                                            JACOB   1610
      CONDUCT = NE*E0*MU                                                JACOB   1611
      RD = D/AREA/CONDUCT                                               JACOB   1612
C                                                                       JACOB   1613
      IF (L0.EQ.0.) GO TO 2                                             JACOB   1614
      PHI(25,25) = 0.                                                   JACOB   1615
      PHI(25,26) = 1.0                                                  JACOB   1616
      PHI(26,25) = -1./L0/C0                                            JACOB   1617
      PHI(26,26) = -(R0 + RD)/L0                                        JACOB   1618
      PHI(26, 2) = NO(26)*RD/NE/L0                                      JACOB   1619
      RETURN                                                            JACOB   1620
C                                                                       JACOB   1621
    2 PHI(25,25) = DIDQ = - 1./C0/(R0 + RD)                             JACOB   1622
      PHI(25, 2) = NO(25)*DIDQ*RD/NE/(R0 + RD)                          JACOB   1623
C                                                                       JACOB   1624
C ..................................................................... JACOB   1625
C                                                                       JACOB   1626
C  THE FOLLOWING MOLECULAR SPECIES (WITH LABELS) WERE INCLUDED --       JACOB   1627
C                                                                       JACOB   1628
C   1   RAD          2   E(-)         3   AR          4   AR*           JACOB   1629
C   5   KR           6   KR*          7   AR**       8   KR**          JACOB   1630
C   9   AR(+)       10   KR(+)       11   AR2(+)     12   KR2(+)        JACOB   1631
C  13   F2          14   F           15   F-         16   AR2*          JACOB   1632
C  17   KR2*        18   ARKR(+)     19   ARKR*      20   ARF*          JACOB   1633
C  21   AR2F*       22   KRF*        23   KR2F*      24   ARKRF*        JACOB   1634
C                                                                       JACOB   1635
C ..................................................................... JACOB   1636
C                                                                       JACOB   1637
      RETURN                                                            JACOB   1638
      END                                                               JACOB   1639
```

Fig. 4.3 (Continued)

```
      SUBROUTINE LEVELS (N1, N2, NO)
C
C ..................................................................
C
C     THIS SUBROUTINE DETERMINES THE POPULATION DENSITIES N1(I), N2(I)
C     OF THE (LOWER AND UPPER) LEVELS INVOLVED IN THE ITH INELASTIC
C     SCATTERING PROCESS INCLUDED IN THE COUPLED E- KINETICS ANALYSIS.
C
C     THE GENERAL KINETICS SYNTHESIS PROGRAM WHICH AUTOMATICALLY GEN-
C     ERATED THIS SUBROUTINE WAS DEVELOPED BY --
C
C              ----------------------------------------
C              I                                      I
C              I   DR. WILLIAM B. LACINA              I
C              I   NORTHROP RESEARCH AND TECHNOLOGY   I
C              I   ONE RESEARCH PARK                  I
C              I   PALOS VERDES PENINSULA, CA 90274   I
C              I   TEL: (213) 377-4811, EXT. 322      I
C              I                                      I
C              ----------------------------------------
C
C ..................................................................
C
      REAL N1(1), N2(1), NO(1)
C
      N1( 1) = NO( 3)
      N2( 1) = NO( 4)
C
      N1( 2) = NO( 5)
      N2( 2) = NO( 6)
C
      N1( 3) = NO( 3)
      N2( 3) = NO( 7)
C
      N1( 4) = NO( 5)
      N2( 4) = NO( 8)
C
      N1( 5) = NO( 4)
      N2( 5) = NO( 7)
C
      N1( 6) = NO( 6)
      N2( 6) = NO( 8)
C
      N1( 7) = NO( 3)
      N2( 7) = 0.
C
      N1( 8) = NO( 5)
      N2( 8) = 0.
C
      N1( 9) = NO( 4)
      N2( 9) = 0.
C
      N1(10) = NO( 6)
      N2(10) = 0.
C
      N1(11) = NO( 7)
      N2(11) = 0.
C
      N1(12) = NO( 8)
      N2(12) = 0.
C
      N1(13) = NO(11)
      N2(13) = 0.
C
      N1(14) = NO(12)
      N2(14) = 0.
C
      N1(15) = NO(13)
      N2(15) = 0.
C
      RETURN
      END
```

Fig. 4.4 (Synthesized) Subroutine LEVELS

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
1	AR + E → AR* + E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
2	KR + E → KR* + E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
3	AR + E → AR** + E	(COMPUTED)	(COMPUTED)	0.1 X CROSS SECTION FOR AR + E → AR* + E IS ASSUME FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
4	KR + E → KR** + E	(COMPUTED)	(COMPUTED)	0.1 X CROSS SECTION FOR KR + E → KR* + E IS ASSUME FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
5	AR* + E → AR** + E	(COMPUTED)	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
6	KR* + E → KR** + E	(COMPUTED)	(COMPUTED)	VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
7	AR + E → AR(+) + E + E	(COMPUTED)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
8	KR + E → KR(+) + E + E	(COMPUTED)		KIEFFER REPORT, P. 16 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
9	AR* + E → AR(+) + E + E	(COMPUTED)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
10	KR* + E → KR(+) + E + E	(COMPUTED)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme.

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
11	AR** + E → AR(+) + E + E	(COMPUTED)		VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
12	KR** + E → KR(+) + E + E	(COMPUTED)		VRIENS CROSS SECTION FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
13	AR2(+) + E → AR* + AR	(COMPUTED)		MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE** FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
14	KR2(+) + E → KR* + KR	(COMPUTED)		OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
15	F2 + E → F + F-	(COMPUTED)		AEROSPACE (PRIVATE COMMUN.) FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE REACTION IS IGNORED -- KR = 0.
16	AR2* + E → AR + AR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
17	KR2* + E → KR + KR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
18	AR + HE- → AR(+) + HE- + E	4.3400E-18		BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV) E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION REVERSE REACTION IS IGNORED -- KR = 0.
19	AR + HE- → AR* + HE-	1.2400E-18	1.2400E-18	(1/3.5) X AR + HE → AR(+) + E + HE
20	KR + HE- → KR(+) + HE- + E	8.0400E-18		BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV) E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION REVERSE REACTION IS IGNORED -- KR = 0.
21	KR + HE- → KR* + HE-	2.3000E-18	2.3000E-18	(1/3.5) X KR + HE → KR(+) + E + HE
22	AR(+) + AR + M → AR2(+) + M	2.0000E-31		W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975) REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
23	AR(+) + KR + M → ARKR(+) + M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
24	KR(+) + KR + M → KR2(+) + M	2.4000E-31		C. J. TRACY, M. J. OSKAM JCP 65, 3387 (1976) REVERSE REACTION IS IGNORED -- KR = 0.
25	KR(+) + AR + M → ARKR(+) + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
26	AR(+) + KR → AR + KR(+)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
27	AR2(+) + KR → KR(+) + AR + AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE REACTION IS IGNORED -- KR = 0.
28	ARKR(+) + KR → KR2(+) + AR	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
29	AR* + AR + M → AR2* + M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974. REVERSE REACTION IS IGNORED -- KR = 0.
30	AR* + KR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
31	KR* + KR + M → KR2* + M	5.5000E-32		HUGHES LASL ASPEN 9/76 REVERSE REACTION IS IGNORED -- KR = 0.
32	KR* + AR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
33	ARKR* + KR → KR2* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
34	AR2(+) + F- → ARF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	AR2(+) + F- → AR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
36	AR(+) + F- → ARF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
37	KR2(+) + F- → KRF* + KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	KR2(+) + F- → KR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
39	KR(+) + F- → KRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
40	ARKR(+) + F- → KRF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
41	ARKR(+) + F- → ARKRF*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
42	KR* + F2 → KRF* + F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
43	AR* + F2 → ARF* + F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
44	AR* + KR → AR + KR*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 63, 4018 (1975) REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
45	KRF* + AR + M → ARKRF* + M	6.0000E-32		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
46	KRF* + KR + M → KR2F* + M	5.0000E-31		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
47	ARF* + AR + M → AR2F* + M	4.0000E-31		AVCO REVERSE REACTION IS IGNORED -- KR = 0.
48	ARF* + KR + M → ARKRF* + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
49	AR2* + KR → AR + AR + KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI) REVERSE REACTION IS IGNORED -- KR = 0.
50	AR2* + AR2* → AR2(+) + AR + AR + E	3.0000E-10		E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
51	ARF* + KR → KRF* + AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
52	AR2* + F → ARF* + AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
53	KR2* + F → KRF* + KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
54	AR2* + F2 → AR2F* + F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
55	ARKR* + F2 → KRF* + AR + F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
56	ARKR* + F2 → ARKRF* + F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
57	KR2* + F2 → KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
58	AR2F* + F2 → AR + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
59	ARKRF* + F2 → AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
60	KR2F* + F2 → KR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
61	ARKRF* + KR → KR2F* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
62	KRF* + F2 → KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
63	ARF* + F2 → AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
64	AR2F* + KR → KRF* + AR + AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR** + M → AR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR** + M → KR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF* → AR + F	3.3000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
68	AR2* → AR + AR	3.8000E+06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
69	ARKR* → AR + KR	3.0000E+06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2* → KR + KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
71	AR2F* → AR + AR + F	2.0000E+08		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
72	ARKRF* → AR + KR + F	5.0000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
73	KR2F* → KR + KR + F	6.7000E+07		SRI REPORT NO. MP 76-99, DEC., 1976 REVERSE REACTION IS IGNORED -- KR = 0.
74	KRF* → KR + F + HNU	1.1000E+08		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP) REVERSE REACTION IS IGNORED -- KR = 0. NO REVERSE REACTION ALLOWED FOR RADIATIVE DECAY.
75	KRF* + RAD → KR + F + RAD	2.0000E-16		LASER TRANSITION: STIMULATED EMISSION X-SECTION REVERSE REACTION IS IGNORED -- KR = 0.
76	F2 + RAD → F + F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F- + RAD → F + E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971) E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
78	KR2F* + RAD → AR* + KR + F	1.0000E-99		CROSS SECTION UNKNOWN REVERSE REACTION IS IGNORED -- KR = 0.
79	AR2(+) + RAD → AR + AR(+)	1.5000E-17		STEVENS (PARK CITY CONFERENCE) REVERSE REACTION IS IGNORED -- KR = 0.
80	KR2(+) + RAD → KR + KR(+)	3.5000E-18		J. WEST (NRTC) REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

OF 80 INPUT REACTIONS SCANNED, 80 WERE RETAINED (MAXIMUM ALLOWED = 200) AND 0 WERE IGNORED FOR REASONS ITEMIZED IN THE TABLE.
OF THOSE RETAINED, 15 REQUIRE RATES FROM AN E- KINETICS ANALYSIS. 24 SEPARATE SPECIES WERE ENCOUNTERED (MAXIMUM ALLOWED = 30).

Fig. 4.5: Summary of input reaction scheme (cont'd).

SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NTYPE = 24
(THIS EDIT PERMITS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

I	GAS(I)	REACTIONS CONTAINING GAS(I)
1	RAD	75, 76, 77, 78, 79, 80,
2	E(-)	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 20, 50 77,
3	AR	1, 3, 7, 13, 16, 18, 19, 22, 25, 26, 27, 28, 29, 32, 33, 34, 40, 44, 45, 47 49, 50, 51, 52, 55, 58, 59, 61, 63, 64, 67, 68, 69, 71, 72, 79,
4	AR*	1, 5, 9, 13, 19, 29, 30, 43, 44, 65, 78,
5	KR	2, 4, 8, 14, 17, 20, 21, 23, 24, 26, 27, 28, 30, 31, 33, 37, 44, 46, 48, 49 51, 53, 59, 60, 61, 62, 64, 69, 70, 72, 73, 74, 75, 78, 80,
6	KR*	2, 6, 10, 14, 21, 31, 32, 42, 44, 49, 66,
7	AR**	3, 5, 11, 65,
8	KR**	4, 6, 12, 66,
9	AR(+)	7, 9, 11, 18, 22, 23, 26, 36, 79,
10	KR(+)	8, 10, 12, 20, 24, 25, 26, 27, 39, 80,
11	AR2(+)	13, 22, 27, 34, 35, 50, 79,
12	KR2(+)	14, 24, 28, 37, 38, 80,
13	F2	15, 42, 43, 54, 55, 56, 57, 58, 59, 60, 62, 63, 76,
14	F	15, 42, 43, 52, 53, 54, 55, 56, 57, 58, 59, 60, 62, 63, 67, 71, 72, 73, 74, 75 76, 77, 78,
15	F-	15, 34, 35, 36, 37, 38, 39, 40, 41, 77,
16	AR2*	16, 29, 49, 50, 52, 54, 68,
17	KR2*	17, 31, 33, 53, 57, 70,
18	ARKR(+)	23, 25, 28, 40, 41,
19	ARKR*	30, 32, 33, 55, 56, 69,

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.6: Cross-reference table between species and reactions.

SUMMARY OF REACTIONS FOR WHICH EACH SPECIES OCCURS: NTYPE = 24
(THIS EDIT PERMITS RAPID DELETION OF ANY SPECIES FROM THE KINETIC SYSTEM)

I	GAS(I)	REACTIONS CONTAINING GAS(I)
20	ARF*	34, 36, 43, 47, 48, 51, 52, 63, 67,
21	AR2F*	35, 47, 54, 58, 64, 71,
22	KRF*	37, 39, 40, 42, 45, 46, 51, 53, 55, 62, 64, 74, 75,
23	KR2F*	38, 46, 57, 60, 61, 73, 78,
24	ARKRF*	41, 45, 48, 56, 59, 61, 72,

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 01/04/79

Fig. 4.6: Cross-reference table between species and reactions (cont'd).

(as indicated in Fig.3.5) or directly (with the control card deck given in Fig. 3.6). Fig. 4.7 shows the "playback" (generated in output by subroutine EDITOR) of the exact input card images of DATA BLOCK 4, which specifies the experimental conditions. The structure of the input deck has been described in Sec. 3.2 and summarized in Tables 3.4 - 3.10.

At the beginning of the output after execution of the analysis, a cover page as shown in Fig. 4.8 (actually, two identical such pages) is generated, containing a block-letter title defined by the header card of DATA BLOCK 1 at the time of program synthesis (cf. Fig. 4.1). As described in Table 3.5, the IO input vector provided by $CONTROL$ entry (cf. Fig. 4.7) is used to specify output option requests. If IO(10) is nonzero, an initial summary of the reaction scheme and its rate constants (as modified by $RATES$ input entry) is generated, shown in Fig. 4.9. (The effect of rate modifications will be illustrated in Sec. 4.3 below.) *Only the first (50 BCD character) line of comments* which appeared in Fig. 4.5 is retained. If IO(8) and IO(9) had been entered nonzero, a tabular summary and plot of all inelastic and momentum transfer electron cross section data (used in the analysis) is provided, as shown in Fig. 4.10 and 4.11. The parameters IO(I), I = 1, 2, . . . , 7 are used to specify the frequency of certain output options described in Table 3.5. Fig. 4.12 - 4.18 are samples of such output corresponding to cycle k = 20 ($t = 200 \times 10^{-9}$ s). The first five of these figures summarize results of the electron kinetics analysis at t = 200 ns, while the sixth (Fig. 4.17) summarizes the molecular kinetic, electrical, and optical parameters.

Note that Fig. 4.17 contains a tabulation of the population densities and their instantaneous rates of change for all of the species. Also shown

is an effective (instantaneous) time constant τ_I for each species I,

$$\tau_I(t)^{-1} = \left| dN_I(t)/dt \right| / N_I(t),$$

which is useful for indication of how rapidly any given species is evolving at any given time. Fig. 4.18 is a (partial) reproduction of output which summarizes the numerical contribution of each kinetic reaction to every species, and is useful for assessing reaction sensitivities. If a particular reaction makes only a negligible contribution under typical conditions of interest, it can easily be deleted in a future version of the program. Since the output format of Fig. 4.12 - 4.18 is essentially self-explanatory, no further description should be necessary.

At the conclusion of the analysis, numerous parameters are plotted or tabulated as a function of time, such as e^--beam current density (Fig. 4.19), intracavity radiation intensity (Fig. 4.20), circuit voltages and power densities (Fig. 4.21), instantaneous net gain coefficient (Fig. 4.22) and medium gain and absorption coefficients (Fig. 4.23), optical and electrical power densities (Fig. 4.24) and energy densities (Fig.4.25), circuit voltages (Fig. 4.26), plasma conductivity and discharge impedance (Fig. 4.27), discharge current density (Fig. 4.28), optically extracted power (Fig. 4.29) and energy (Fig. 4.30) density and efficiency, and the population densities (and rates of change) for miscellaneous species as requested (Fig. 4.31 - 4.35).

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                              (DATE: 01/12/79)

CARD            1         2         3         4         5         6         7         8
 NO.    12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------------

  1 ...  $CONTROL          IO(1) = 10,20,20,20,10,10,20,0,0,1,
  2 ...                    EMAX = 20.,
  3 ...                    NCYCLE = 100$
  4 ...  $PARAM            TPULSE = 1.0E-06,
  5 ...                    ATM = 2.0$
  6 ...  $OPTICAL          REFLECT = 70.,
  7 ...                    LOSS = 0.,
  8 ...                    AREA = 25.,
  9 ...                    CAVITY = 130.,
 10 ...                    LENGTH = 75.0$
 11 ...  $EBEAM            JBEAM = 10.0,
 12 ...                    ENERGY = 300.,
 13 ...                    UB = 20.,
 14 ...                    TB(1) = 0., 50., 100., 150., 200., 250., 300.,
 15 ...                            350., 400., 450., 500., 550., 600., 650.,
 16 ...                            700., 750., 800., 850., 900., 950., 1000.,
 17 ...                    UNITS = 1.0E-09,
 18 ...                    JB(1) = 0., .82, 1., 1., .9, .85, .77, .73, .69,
 19 ...                            .67, .69, .72, .75, .75, .72, .65, .42, .2,
 20 ...                            .05, .02, 0.,
 21 ...                    FACTOR = 2.0$
 22 ...  $CIRCUIT          CAPAC = 1.00E-06,
 23 ...                    INDUCT = 200.E-09,
 24 ...                    RESIST = 0.,
 25 ...                    KVOLT = 50.,
 26 ...                    AREA = 2000.,
 27 ...                    DIST = 10.$
 28 ...  $RATES $
 29 ...AR            89.9                40.
 30 ...KR            10.0                84.
 31 ...F2             0.1                38.          PLOT
 32 ...AR*                      11.5                 PLOT
 33 ...KR*                       9.9                 PLOT
 34 ...AR2(+)                   13.0                 PLOT
 35 ...KR2(+)                   11.8                 PLOT
 36 ...ARKR(+)                  12.4
 37 ...AR**                     13.5
 38 ...AR(+)                    15.8                 PLOT
 39 ...KR**                     11.5
 40 ...KR(+)                    14.4                 PLOT
-------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8

                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                              (DATE: 01/12/79)

CARD            1         2         3         4         5         6         7         8
 NO.    12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------------

 41 ...AR F*                    6.5                  PLOT
 42 ...KR F*                    5.0                  PLOT
 43 ...AR2*                     9.5
 44 ...KR2*                     8.2
 45 ...AR2F*                    5.0
 46 ...ARKRF*                   4.0
 47 ...KR2F*                    3.0
 48 ...ARKR*                    8.8
 49 ...F-                                            PLOT
 50 ...E(-)                                          PLOT
-------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.7: DATA BLOCK 4 card input of numerical control values, experimental parameters, modification of rate constants, and initialization of species.

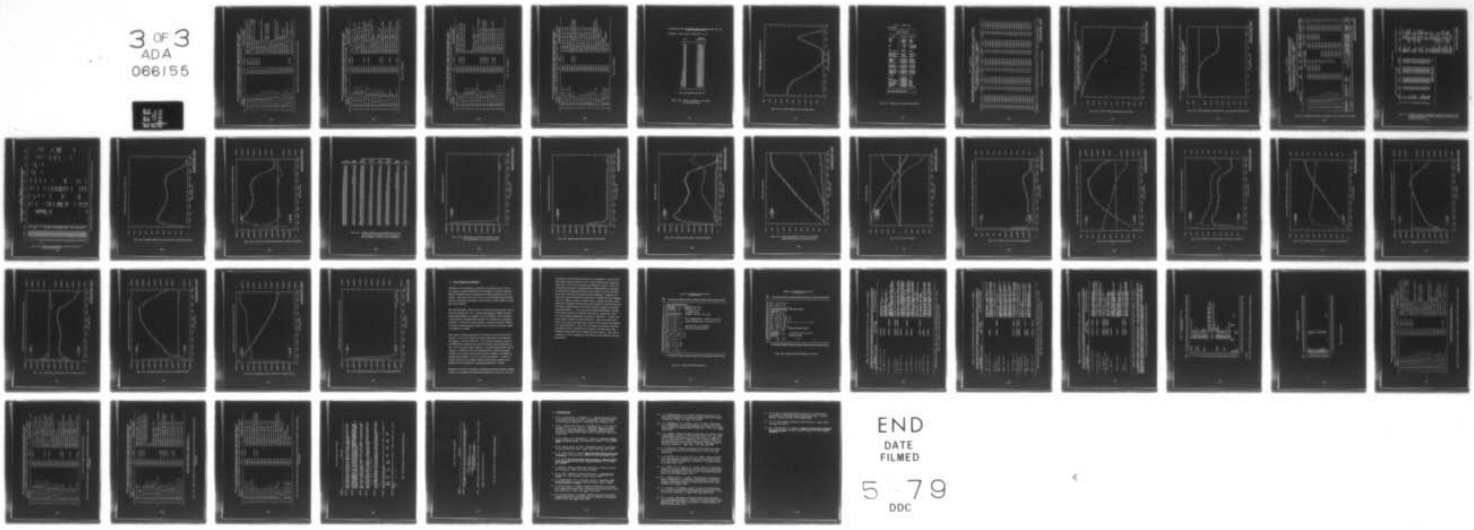
```
XX      XX    XXXXXXXX    XXXXXXXXX    XXXXXXXXXX   XX      XX   XXXXXXXXX     XXXXXXXX    XXXXXXXXX
XXX     XX   XXXXXXXXXX   XXXXXXXXXX   XXXXXXXXXX   XX      XX   XXXXXXXXXX   XXXXXXXXXX   XXXXXXXXXX
XXXX    XX   XX      XX   XX      XX      XX        XX      XX   XX      XX   XX      XX   XX      XX
XX XX   XX   XX      XX   XX      XX      XX        XX      XX   XX      XX   XX      XX   XX      XX
XX  XX  XX   XX      XX   XXXXXXXXX       XX        XXXXXXXXXX   XXXXXXXXXX   XX      XX   XXXXXXXXXX
XX  XX  XX   XX      XX   XXXXXXXXX       XX        XXXXXXXXXX   XXXXXXXXX    XX      XX   XXXXXXXXX
XX   XX XX   XX      XX   XX   XX         XX        XX      XX   XX   XX      XX      XX   XX
XX    XXXX   XX      XX   XX    XX        XX        XX      XX   XX    XX     XX      XX   XX
XX     XXX   XXXXXXXXXX   XX     XX       XX        XX      XX   XX     XX    XXXXXXXXXX   XX
XX      XX    XXXXXXXX    XX      XX      XX        XX      XX   XX      XX    XXXXXXXX    XX

XX      XX   XXXXXXXXXX   XXXXXXXXXX                XX           XXXXXXXX    XXXXXXXX   XXXXXXXXXX   XXXXXXXXX
XX     XX    XXXXXXXXXX   XXXXXXXXXX                XX          XXXXXXXXXX  XXXXXXXXXX  XXXXXXXXXX   XXXXXXXXXX
XX   XX      XX      XX   XX                        XX          XX      XX  XX      XX  XX            XX      XX
XX XX        XX      XX   XX                        XX          XX      XX  XX          XX            XX      XX
XXXXX        XXXXXXXXXX   XXXXXX                    XX          XX      XX  XXXXXXXXXX  XXXXXX       XXXXXXXXXX
XX  XX       XXXXXXXXXX   XXXXXX                    XX          XXXXXXXXXX   XXXXXXXXX  XXXXXX       XXXXXXXXX
XX   XX      XX    XX     XX                        XX          XXXXXXXXXX             XX   XX            XX    XX
XX    XX     XX     XX    XX                        XX          XX      XX  XX      XX  XX            XX     XX
XX     XX    XX      XX   XX                        XXXXXXXXXX  XX      XX  XXXXXXXXXX  XXXXXXXXXX   XX      XX
XX      XX   XX      XX   XX                        XXXXXXXXXX  XX      XX   XXXXXXXX   XXXXXXXXXX   XX      XX

XX      XX    XXXXXXXX    XX      XX   XXXXXXXXXX   XXXXXXXXXX   XXXXXXXX    XXXXXXXX    XXXXXXXX
XX     XX     XXXXXXXX    XXX     XX   XXXXXXXXXX   XXXXXXXXXX   XXXXXXXX   XXXXXXXXXX  XXXXXXXXXX
XX   XX           XX      XXXX    XX   XX               XX           XX       XX      XX  XX      XX
XX XX             XX      XX XX   XX   XX               XX           XX       XX          XX
XXXXX             XX      XX  XX  XX   XXXXXX           XX           XX       XX          XXXXXXXXX
XX  XX            XX      XX  XX  XX   XXXXXX           XX           XX       XX           XXXXXXXX
XX   XX           XX      XX   XX XX   XX               XX           XX       XX                  XX
XX    XX          XX      XX    XXXX   XX               XX           XX       XX      XX  XX      XX
XX     XX    XXXXXXXX    XX     XXX   XXXXXXXXXX       XX        XXXXXXXX  XXXXXXXXXX  XXXXXXXXXX
XX      XX   XXXXXXXX    XX      XX   XXXXXXXXXX       XX        XXXXXXXX    XXXXXXXX    XXXXXXXX
```

```
*****************************************
*                                       *
*                                       *
*   THIS CODE WAS DEVELOPED BY          *
*                                       *
*       DR. WILLIAM B. LACINA           *
*       NORTHROP RESEARCH AND TECHNOLOGY *
*       ONE RESEARCH PARK               *
*       PALOS VERDES PENINSULA, CA 90274 *
*       TEL: (213) 377-4811, EXT. 322   *
*                                       *
*                                       *
*****************************************
```

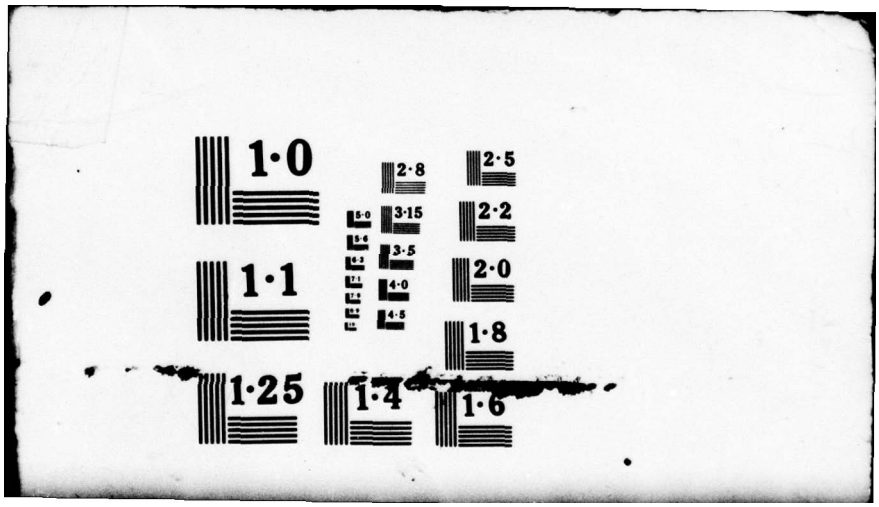
Fig. 4.8: Cover page, generated at beginning of each output, with a block-letter title defined by the header card of DATA BLOCK 1 at time of program synthesis.

AD-A066 155 NORTHROP RESEARCH AND TECHNOLOGY CENTER PALOS VERDES --ETC F/G 20/5
THEORETICAL MODELING OF MOLECULAR AND ELECTRON KINETIC PROCESSE--ETC(U)
JAN 79 W B LACINA N00014-78-C-0499
UNCLASSIFIED NRTC-79-7R-VOL-1 NL

3 OF 3
ADA
066155



END
DATE
FILMED
5 79
DDC


1·0
2·8
2·5
5·0
3·15
2·2
3·5
2·0
1·1
4·0
4·5
1·8
1·25
1·4
1·6

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
1	AR + E → AR* + E	VSIG(1, 1)	VSIG(2, 1)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
2	KR + E → KR* + E	VSIG(1, 2)	VSIG(2, 2)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
3	AR + E → AR** + E	VSIG(1, 3)	VSIG(2, 3)	0.1 X CROSS SECTION FOR AR + E → AR* + E IS ASSUME
4	KR + E → KR** + E	VSIG(1, 4)	VSIG(2, 4)	0.1 X CROSS SECTION FOR KR + E → KR* + E IS ASSUME
5	AR* + E → AR** + E	VSIG(1, 5)	VSIG(2, 5)	VRIENS CROSS SECTION
6	KR* + E → KR** + E	VSIG(1, 6)	VSIG(2, 6)	VRIENS CROSS SECTION
7	AR + E → AR(+) + E + E	VSIG(1, 7)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43
8	KR + E → KR(+) + E + E	VSIG(1, 8)		KIEFFER REPORT, P. 16
9	AR* + E → AR(+) + E + E	VSIG(1, 9)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
10	KR* + E → KR(+) + E + E	VSIG(1,10)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
11	AR** + E → AR(+) + E + E	VSIG(1,11)		VRIENS CROSS SECTION
12	KR** + E → KR(+) + E + E	VSIG(1,12)		VRIENS CROSS SECTION
13	AR2(+) + E → AR* + AR	VSIG(1,13)		MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE**
14	KR2(+) + E → KR* + KR	VSIG(1,14)		OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW.
15	F2 + E → F + F-	VSIG(1,15)		AEROSPACE (PRIVATE COMMUN.)
16	AR2* + E → AR + AR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
17	KR2* + E → KR + KR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
18	AR + HE- → AR(+) + HE- + E	4.3400E-18		BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV)
19	AR + HE- → AR* + HE-	1.2400E-18	1.2400E-18	(1/3.5) X AR + HE → AR(+) + E + HE
20	KR + HE- → KR(+) + HE- + E	8.0400E-18		BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV)

Fig. 4.9: Summary of rate constants used for execution.

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
21	KR + HE- → KR* + HE-	2.3000E-18	2.3000E-18	(1/3.5) X KR + HE → KR(+) + E + HE
22	AR(+) + AR + M → AR2(+) + M	2.0000E-31		W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975)
23	AR(+) + KR + M → ARKR(+) + M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
24	KR(+) + KR + M → KR2(+) + M	2.4000E-31		C. J. TRACY, H. J. OSKAM JCP 65, 3387 (1976)
25	KR(+) + AR + M → ARKR(+) + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
26	AR(+) + KR → AR + KR(+)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
27	AR2(+) + KR → KR(+) + AR + AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
28	ARKR(+) + KR → KR2(+) + AR	3.2000E-10	X E(-E/KT)	BOHME ET AL. J. CHEM. PHYS. 52, 5094 (1970)
29	AR* + AR + M → AR2* + M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL. SRI REPORT, 1974.
30	AR* + KR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
31	KR* + KR + M → KR2* + M	5.5000E-32		HUGHES LASL ASPEN 9/76
32	KR* + AR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
33	ARKR* + KR → KR2* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
34	AR2(+) + F- → ARF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
35	AR2(+) + F- → AR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
36	AR(+) + F- → ARF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
37	KR2(+) + F- → KRF* + KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
38	KR2(+) + F- → KR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
39	KR(+) + F- → KRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
40	ARKR(+) + F- → KRF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

Fig. 4.9: Continued

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
41	ARKR(+) + F- → ARKRF*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
42	KR* + F2 → KRF* + F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
43	AR* + F2 → ARF* + F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
44	AR* + KR → AR + KR*	6.2000E-12	X E(-E/KT)	PIPER, SETSER, CLYNE, JCP 63, 4018 (1975)
45	KRF* + AR + M → ARKRF* + M	6.0000E-32		AVCO
46	KRF* + KR + M → KR2F* + M	5.0000E-31		AVCO
47	ARF* + AR + M → AR2F* + M	4.0000E-31		AVCO
48	ARF* + KR + M → ARKRF* + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
49	AR2* + KR → AR + AR + KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI)
50	AR2* + AR2* → AR2(+) + AR + AR + E	3.0000E-10		E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
51	ARF* + KR → KRF* + AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
52	AR2* + F → ARF* + AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
53	KR2* + F → KRF* + KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
54	AR2* + F2 → AR2F* + F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
55	ARKR* + F2 → KRF* + AR + F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976
56	ARKR* + F2 → ARKRF* + F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
57	KR2* + F2 → KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
58	AR2F* + F2 → AR + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
59	ARKRF* + F2 → AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
60	KR2F* + F2 → KR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976

Fig. 4.9: Continued

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
61	ARKRF* + KR → KR2F* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
62	KRF* + F2 → KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
63	ARF* + F2 → AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
64	AR2F* + KR → KRF* + AR + AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR** + M → AR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR** + M → KR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF* → AR + F	3.3000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
68	AR2* → AR + AR	3.8000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
69	ARKR* → AR + KR	3.0000E+06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2* → KR + KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
71	AR2F* → AR + AR + F	2.0000E+08		SRI REPORT NO. MP 76-99, DEC., 1976
72	ARKRF* → AR + KR + F	5.0000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
73	KR2F* → KR + KR + F	6.7000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
74	KRF* → KR + F + HNU	1.1000E+08		R. BURNHAM, S. S. SEARLES (SUBMITTED TO JCP)
75	KRF* + RAD → KR + F + RAD	2.0000E-16		LASER TRANSITION: STIMULATED EMISSION X-SECTION
76	F2 + RAD → F + F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F- + RAD → F + E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971)
78	KR2F* + RAD → AR* + KR + F	1.0000E-99		CROSS SECTION UNKNOWN
79	AR2(+) + RAD → AR + AR(+)	1.5000E-17		STEVENS (PARK CITY CONFERENCE)
80	KR2(+) + RAD → KR + KR(+)	3.5000E-18		J. WEST (NRTC)

Fig. 4.9: Continued

CROSS SECTION (UNITS OF 1.000E-16 CM2) VS ELECTRON ENERGY (EV) FOR MOMENTUM TRANSFER FOR KR

REFERENCE -- FROST, PHELPS: KIEFFER REPT., P. 15

U (EV)	SIGMA(U) (1.0E-16 CM2)
0.000	3.070E+01
.010	2.600E+01
.020	1.967E+01
.030	1.600E+01
.050	1.143E+01
.070	9.000E+00
.100	6.800E+00
.130	5.330E+00
.160	3.970E+00
.200	2.470E+00
.240	1.620E+00
.280	1.130E+00
.320	8.700E-01
.360	7.270E-01
.400	6.200E-01
.470	5.400E-01
.560	5.000E-01
.700	5.000E-01
.840	5.400E-01
1.000	6.170E-01
1.300	8.670E-01
1.600	1.320E+00
2.200	2.530E+00
3.000	4.840E+00
5.000	1.020E+01
7.000	1.500E+01
10.000	1.930E+01
12.000	2.200E+01
20.000	1.800E+01
23.000	1.500E+01
30.000	1.000E+01
40.000	5.000E+00

(DATA WAS SUBMITTED ON 03/01/77)

Fig. 4.10: Tabular summary of electron cross section data.

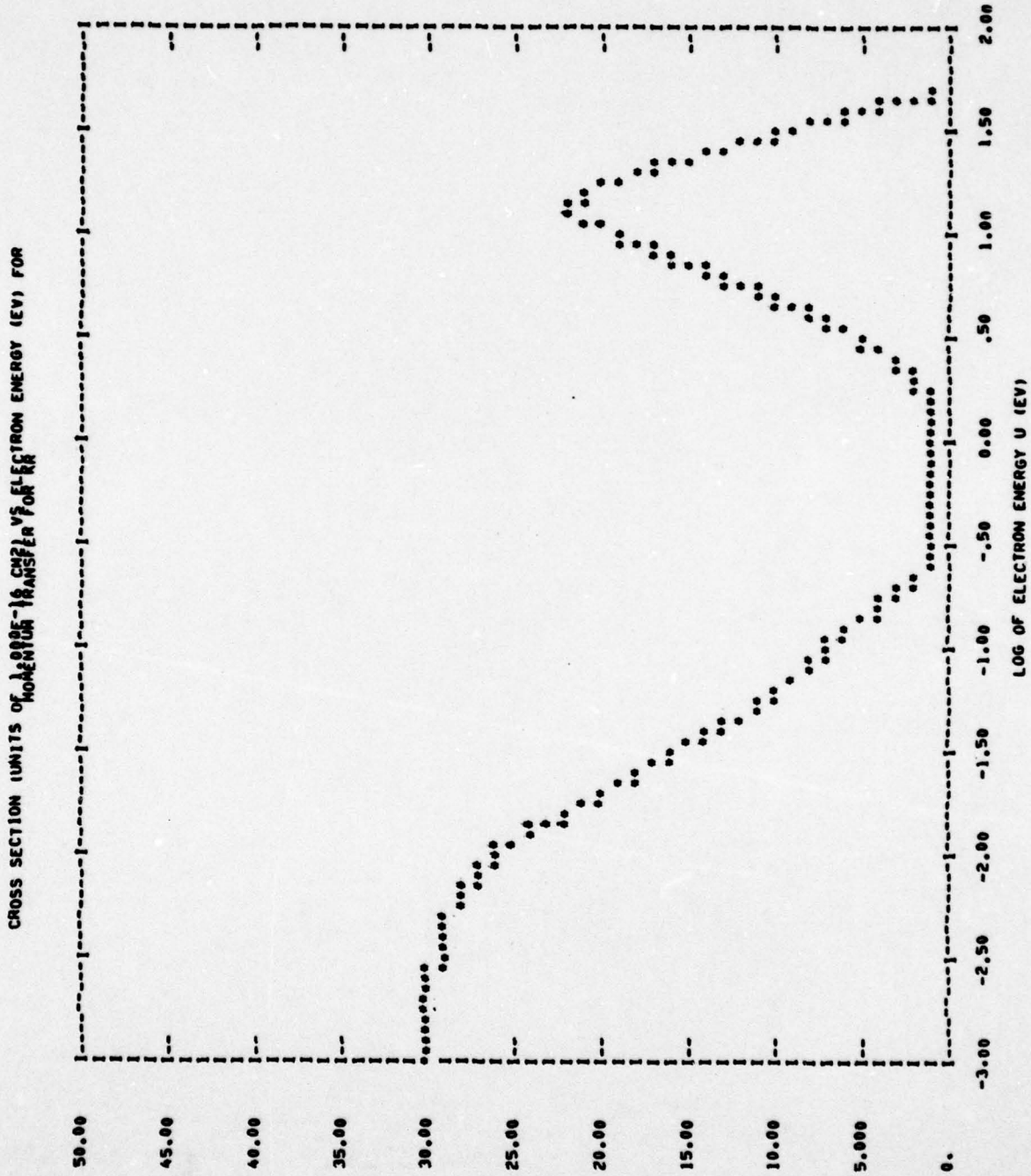


Fig. 4.11: Plot of electron cross section data.

```
          TIME T =  2.000E-07 SEC

GAS MIXTURE --

  AR /KR /F2  =  89.90 / 10.00 /   .10

              PLASMA PARAMETERS

-----------------------------------------

  E (FIELD)     =  8.3123E+02   VOLT/CM

  TMOL          =     300.      DEG K
  NMOL          =  4.8893E+19   CM-3
  PTOT          =    1520.0     TORR
                =     2.00      ATM

  E/N           =  1.7001E-17   VOLT CM2
  E/P           =      .55      V/CM/TORR
                =      .42      KV/CM/ATM

  <U>           =    3.087      EV
  TE = 2<U>/3K  =    23889.     DEG K

  DIFFUSION D   =   2131.97     CM2/SEC
  MOBILITY MU   =    646.9      CM2/VOLT/S
  EK = D/MU     =    3.296      EV
  VDRIFT =MU*E  =  5.3772E+05   CM/SEC

  CONDUCT/NE    =  1.0363E-16   CM2/OHM
  CONDUCT       =  2.5572E-02   /OHM-CM
  RHO*NE        =  9.6495E+15   OHM/CM2
  J/NE = E*VD   =  8.6142E-14   AMP CM/EL

  DISCHARGE     =  1.7669E+04   WATT/CM3
  DEPOSITION    =  4.1411E+04   WATT/CM3
  TOTAL POWER   =  5.9080E+04   WATT/CM3

  INELASTIC     =  4.4363E+04   WATT/CM3
  ELASTIC HEAT  =  1.4642E+04   WATT/CM3
  E<U>DNE/DT    =  3.6592E+02   WATT/CM3
  POWER DISS    =  5.9371E+04   WATT/CM3

  NU(MOM)       =  2.8272E+12   SEC-1

  NE            =  2.4676E+14   CM-3
  NE/NMOL       =  5.0468E-06
  S(U = 0)/NE   =  9.6958E+06   SEC-1
  S(U > 0)/NE   =  1.0476E+08   SEC-1
  NU(IONIZE)    =  2.0009E+07   SEC-1
  NU(ATT,REC)   =  1.3146E+08   SEC-1
  DNE/DT/NE     =  2.9988E+06   SEC-1
  DNE/DT        =  7.3996E+20   CM-3/SEC

-----------------------------------------

CALCULATION PARAMETERS USED:
MESH = 500. EMAX = 20.00 EV. DE = .040 EV.
```

Fig. 4.12: Summary of plasma parameters.

TIME T = 2.000E-07 SEC

NORMALIZED ELECTRON DISTRIBUTION FUNCTION F(U), IN UNITS OF EV**(-3/2), WITH OUTPUT AT .200 EV INTERVALS.
THE ELECTRON ENERGY RANGE [0, 20.00] EV WAS SUBDIVIDED INTO 500 INTERVALS, GIVING A RESOLUTION = .040 EV.

E/NTOT = 1.700E-17 VOLT CM2 = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATM
FRACTIONAL IONIZATION = NE/NTOT = 5.047E-06, NE = 2.468E+14 CM-3
AR /KR /F2 = 89.90 / 10.00 / .10, TMOL = 300. DEG K

U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)	U(EV)	F(U)
0.000	2.37257E-01	.200	2.26884E-01	.400	2.25926E-01	.600	2.21737E-01	.800	2.14309E-01
1.000	2.04916E-01	1.200	1.94431E-01	1.400	1.83417E-01	1.600	1.72206E-01	1.800	1.61055E-01
2.000	1.50173E-01	2.200	1.39645E-01	2.400	1.29552E-01	2.600	1.19935E-01	2.800	1.10814E-01
3.000	1.02198E-01	3.200	9.40991E-02	3.400	8.65108E-02	3.600	7.94080E-02	3.800	7.27663E-02
4.000	6.65624E-02	4.200	6.07721E-02	4.400	5.53767E-02	4.600	5.03587E-02	4.800	4.56974E-02
5.000	4.13812E-02	5.200	3.74050E-02	5.400	3.37552E-02	5.600	3.04081E-02	5.800	2.73422E-02
6.000	2.45369E-02	6.200	2.19739E-02	6.400	1.96351E-02	6.600	1.75025E-02	6.800	1.55594E-02
7.000	1.37908E-02	7.200	1.21776E-02	7.400	1.07070E-02	7.600	9.37284E-03	7.800	8.16836E-03
8.000	7.08600E-03	8.200	6.12156E-03	8.400	5.26789E-03	8.600	4.51402E-03	8.800	3.85085E-03
9.000	3.26876E-03	9.200	2.75864E-03	9.400	2.31228E-03	9.600	1.92192E-03	9.800	1.58102E-03
10.000	1.28370E-03	10.200	1.03001E-03	10.400	8.20086E-04	10.600	6.48637E-04	10.800	5.07181E-04
11.000	3.91099E-04	11.200	2.96681E-04	11.400	2.19807E-04	11.600	1.58013E-04	11.800	1.11797E-04
12.000	7.86320E-05	12.200	5.60808E-05	12.400	4.08831E-05	12.600	3.07529E-05	12.800	2.40876E-05
13.000	1.97079E-05	13.200	1.68346E-05	13.400	1.47187E-05	13.600	1.29080E-05	13.800	1.13089E-05
14.000	9.93381E-06	14.200	8.72439E-06	14.400	7.65515E-06	14.600	6.71722E-06	14.800	5.98548E-06
15.000	5.41339E-06	15.200	4.97300E-06	15.400	4.60246E-06	15.600	4.26121E-06	15.800	3.90958E-06
16.000	3.52906E-06	16.200	3.17339E-06	16.400	2.85857E-06	16.600	2.58305E-06	16.800	2.34151E-06
17.000	2.12760E-06	17.200	1.93594E-06	17.400	1.76904E-06	17.600	1.62412E-06	17.800	1.49760E-06
18.000	1.38639E-06	18.200	1.28789E-06	18.400	1.20051E-06	18.600	1.12281E-06	18.800	1.05335E-06
19.000	9.90760E-07	19.200	9.33893E-07	19.400	8.82282E-07	19.600	8.33521E-07	19.800	7.62625E-07
20.000	3.18267E-07								

F(U) CONVERGED IN 1.8 SEC, IN 12 ITERATIONS; MAXIMUM RELATIVE CHANGE IN LAST ITERATION < 4.530E-04; POWER BALANCE ACCURACY = .20 %.

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Fig. 4.13: Tabular electron distribution.

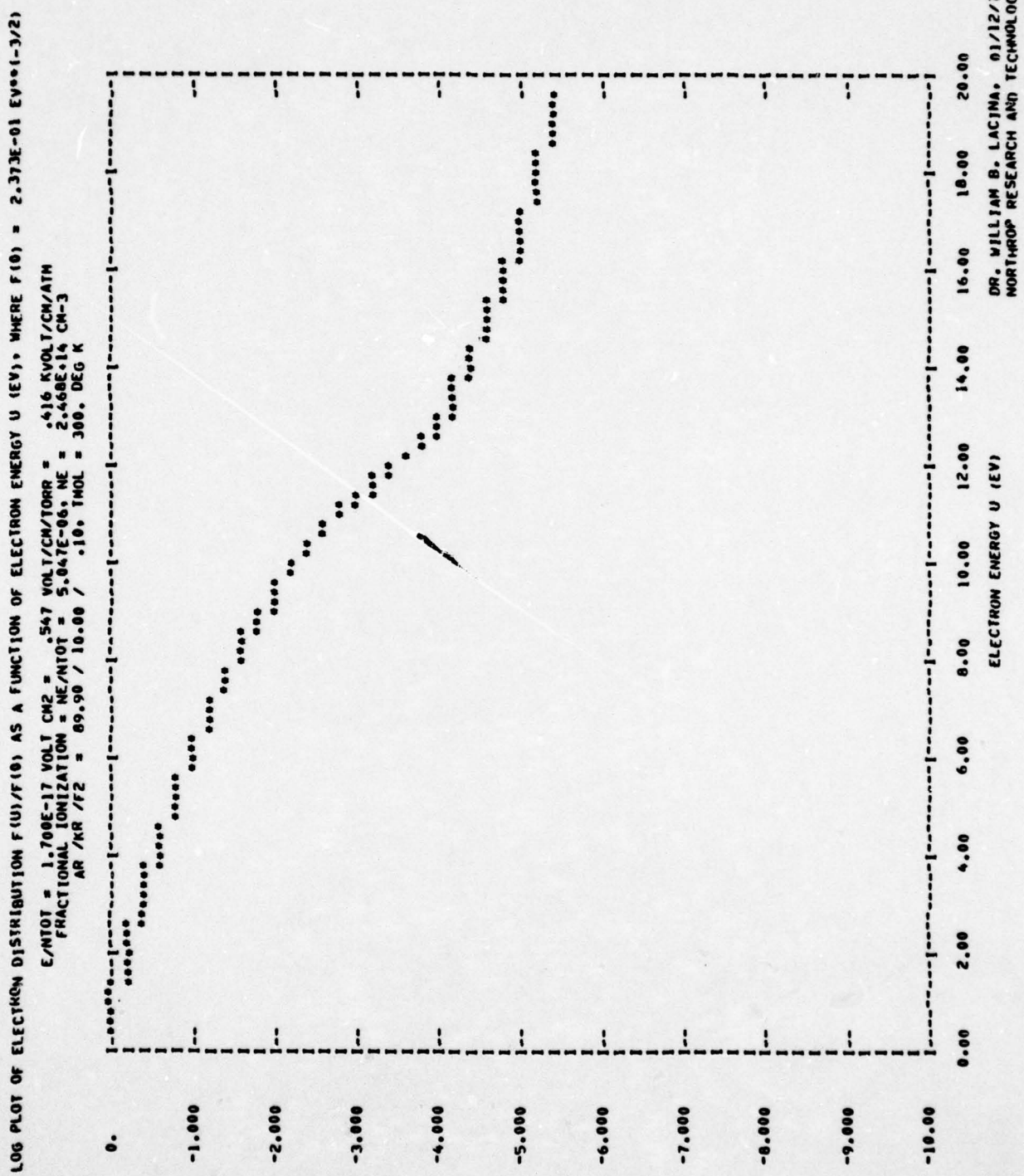

Fig. 4.14: Plot of electron distribution function.

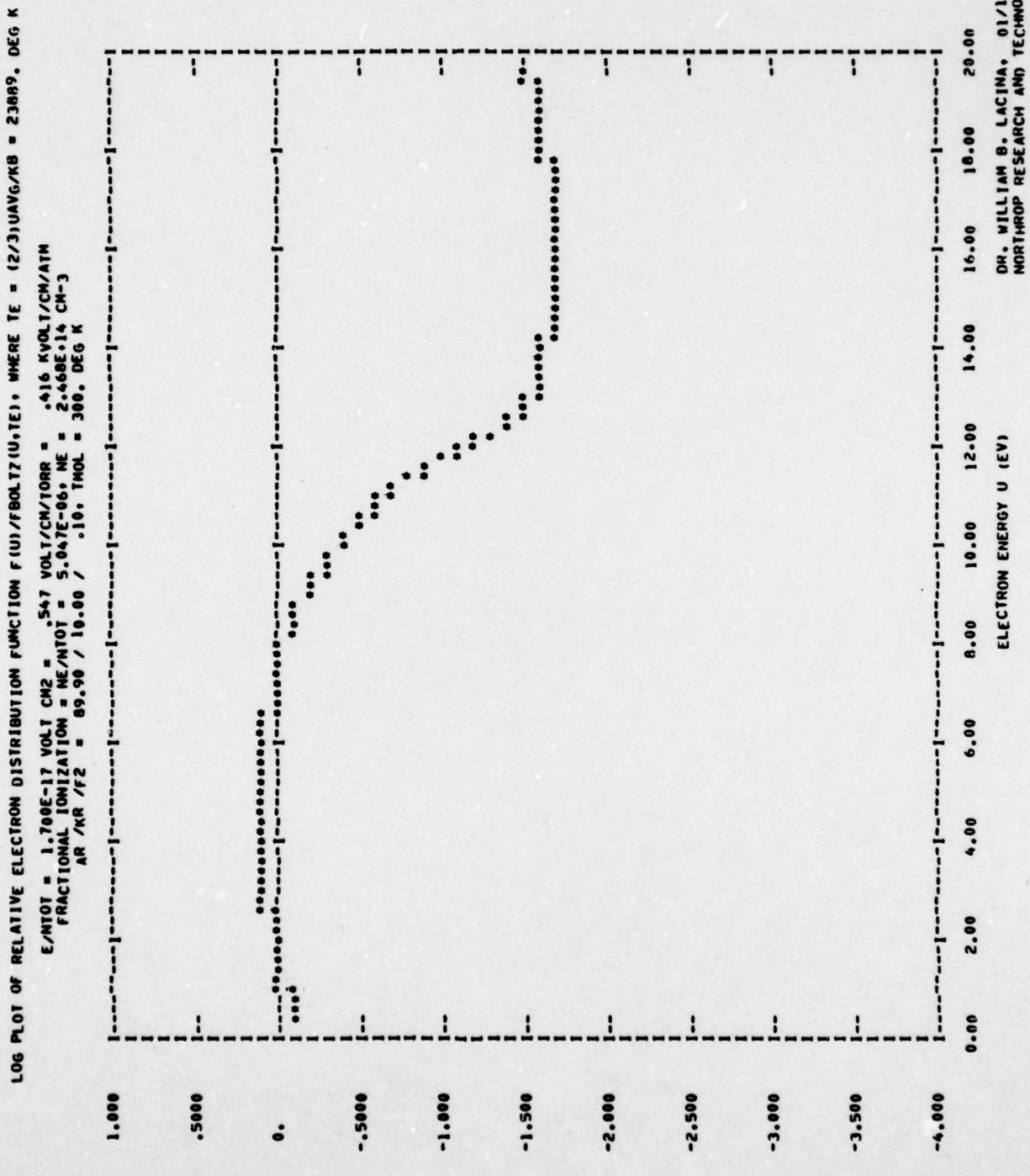

Fig. 4.15: Plot of electron distribution, normalized to Maxwellian.

TIME T = 2.000E-07 SEC

PLASMA KINETICS ANALYSIS WITH SUMMARY OF ELECTRON PARAMETERS, COLLISION RATES,
AND POWER BALANCE FOR ALL ELASTIC AND INELASTIC COLLISION PROCESSES INCLUDED

E/NTOT = 1.700E-17 VOLT CM2 = .547 VOLT/CM/TORR = .416 KVOLT/CM/ATM
FRACTIONAL IONIZATION = NE/NTOT = 5.047E-06, NE = 2.468E+14 CM-3
AR /KR /F2 = 89.90 / 10.00 / .10, TMOL = 300. DEG K

U(AVG) = 3.087 EV, TE = 23889. DEG K, VD = 5.38E+05 CM/SEC, MU = 6.47E+02 CM2/VOLT/SEC

J	REACTION(J) A + E(-) → B + E(-)	N(A) (CM-3)	N(B) (CM-3)	U(J) (EV)	DNE/DT/NE (SEC-1)	<VSIG(A→B)> (CM3/SEC)	<VSIG(B→A)> (CM3/SEC)	(NET) POWER (WATT/CM3)	PERCENT POWER
				S(U > 0)/NE = 1.048E+08			MOMENTUM TRANSFER =	1.464E+04	24.78
				S(U = 0)/NE = 9.696E+06					
1	AR + E → AR* + E	4.395E+19	1.582E+14	11.50		7.084E-13	7.610E-09	1.361E+04	23.03
2	KR + E → KR* + E	4.888E+18	2.528E+14	9.90		4.542E-12	9.396E-09	7.759E+03	13.13
3	AR + E → AR** + E	4.395E+19	3.331E+12	13.50		2.244E-14	7.606E-10	5.250E+02	.89
4	KR + E → KR** + E	4.888E+18	5.876E+12	11.50		5.612E-14	7.028E-10	1.228E+02	.21
5	AR* + E → AR** + E	1.582E+14	3.331E+12	2.00		4.402E-07	1.079E-06	5.221E+03	8.84
6	KR* + E → KR** + E	2.528E+14	5.876E+12	1.60		4.908E-07	9.900E-07	7.480E+03	12.66
7	AR + E → AR(+) + E + E	4.395E+19		15.80	6.771E+06	1.540E-13		4.229E+03	7.16
8	KR + E → KR(+) + E + E	4.888E+18		14.40	2.952E+06	6.039E-13		1.680E+03	2.84
9	AR* + E → AR(+) + E + E	1.582E+14		4.30	3.176E+06	2.008E-08		5.398E+02	.91
10	KR* + E → KR(+) + E + E	2.528E+14		4.50	5.858E+06	2.317E-08		1.042E+03	1.76
11	AR** + E → AR(+) + E + E	3.331E+12		2.30	2.796E+05	8.394E-08		2.542E+01	.04
12	KR** + E → KR(+) + E + E	5.876E+12		2.90	9.740E+05	1.658E-07		1.117E+02	.19
13	AR2(+) + E → AR* + AR	3.792E+12			-1.900E+05	5.010E-08		1.489E+01	.03
14	KR2(+) + E → KR* + KR	1.962E+14			-1.474E+07	7.516E-08		1.155E+03	1.95
15	F2 + E → F + F-	3.915E+16			-1.165E+08	2.976E-09		8.490E+02	1.44

DISCHARGE POWER = 1.767E+04 WATT/CM3 29.91 %,
SOURCE DEPOSITION = 4.141E+04 WATT/CM3 70.09 %,
TOTAL ELECTRICAL = 5.908E+04 WATT/CM3 100.00 %,

POWER INTO INELASTIC E-MOLECULE COLLISIONS = 4.436E+04 75.09 %
ELASTIC E-MOLECULE HEATING = 1.464E+04 24.78 %
D/DT(STORED ELECTRON KINETIC ENERGY) = E<U>DNE/DT = 3.659E+02 .62 %
E-E POWER TRANSFER DISCREPANCY = -1.713E+02 -.29 %
TOTAL POWER INTO COLLISIONS, HEATING, STORAGE = 5.920E+04 100.20 %

F(U) CONVERGED IN 1.8 SEC, IN 12 ITERATIONS; MAXIMUM RELATIVE CHANGE IN LAST ITERATION < 4.530E-04; POWER BALANCE ACCURACY = .20 %.

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Fig. 4.16: Tabular summary of collision rates and power partition.

TIME T = 2.000E-07 SEC

POPULATION DENSITIES AND RATES OF CHANGE

I	SPECIES NAME	E(I) (EV)	N(I) (CM-3)	DN(I)/DT (CM-3/SEC)	TAU(I) 1.0E-09 SEC
1	RAD	.00	1.796E+14	-2.735E+20	656.69
2	E(-)	3.09	2.468E+14	7.400E+20	333.47
3	AR	0.00	4.395E+19	4.056E+20	1.08E+08
4	AR*	11.50	1.582E+14	-4.525E+20	349.58
5	KR	0.00	4.888E+18	-2.001E+20	2.44E+07
6	KR*	9.90	2.528E+14	-1.321E+20	1913.65
7	AR**	13.50	3.331E+12	1.832E+20	18.19
8	KR**	11.50	5.876E+12	2.791E+20	21.06
9	AR(+)	15.80	3.388E+13	-7.757E+19	436.81
10	KR(+)	14.40	8.307E+13	-4.943E+19	1680.66
11	AR2(+)	13.00	3.792E+12	-4.756E+18	797.34
12	KR2(+)	11.80	1.962E+14	1.936E+20	1013.36
13	F2	0.00	3.915E+16	-4.643E+22	843.25
14	F	0.00	1.922E+16	9.361E+22	205.31
15	F-	0.00	8.222E+13	-6.878E+20	119.54
16	AR2*	9.50	7.830E+12	-6.812E+18	1149.38
17	KR2*	8.20	1.935E+14	-9.538E+19	2029.03
18	ARKR(+)	12.40	1.208E+13	-9.677E+18	1248.25
19	ARKR*	8.80	1.102E+13	5.240E+18	2102.31
20	ARF*	6.50	4.525E+12	-9.489E+18	476.85
21	AR2F*	5.00	5.678E+12	-1.118E+19	507.71
22	KRF*	5.00	2.032E+13	4.689E+18	4334.34
23	KR2F*	3.00	1.474E+14	-4.736E+19	3112.68
24	ARKRF*	4.00	5.803E+12	7.128E+17	8141.54

INTEGRATION STEP SIZE = 2.619
ORDER OF INTEGRATION = 3

ELECTRICAL AND OPTICAL PARAMETERS

PARAMETER		VALUE	UNITS
JBEAM	=	9.00	AMP/CM2
DEPOSITION	=	2.00	
ENERGY	=	300.	KEV
DVDX	=	14.66	KV/CM
P(BEAM)	=	131.92	KW/CM3
S(U > 0)	=	2.585E+22	CM-3/SEC
S(U = 0)	=	2.393E+21	CM-3/SEC
AREA	=	2000.00	CM2
DIST	=	10.00	CM
CONDUCT	=	2.557E-02	/OHM/CM
R(DISCH)	=	1.955E-01	OHM
Q	=	4.547E-02	COULOMB
I(DISCH)	=	4.352E+04	AMP
J(DISCH)	=	2.126E+01	AMP/CM2
ESUS	=	.831	KVOLT/CM
ESUS*JSUS	=	17.67	KW/CM3
Q/C	=	45.467	KVOLT
V(DISCH)	=	8.312	KVOLT
L*DI/DT	=	37.155	KVOLT
REFLECT	=	70.00	%
LOSS	=	0.00	%/PASS
T(CAVITY)	=	24.3	NS
L(CAVITY)	=	130.00	CM
LENGTH	=	75.00	CM
OMEGA/4/PI	=	1.177E-04	
THRESH	=	2.378E-03	CM-1
NET GAIN	=	2.290E-03	CM-1
LASER GAIN	=	4.065E-03	CM-1
ABSORPTION	=	1.775E-03	CM-1
INTENSITY	=	4.316E+06	WATT/CM2
OPTICAL	=	10.26	KW/CM3
EFFICIENCY	=	.01	%
E<U>DNE/DT	=	3.659E-01	KW/CM3
DE(TOT)/DT	=	9.371E-02	KW/CM3
E(TOT)	=	1.894E-03	J/CM3
HEAT + SP	=	1.392E+02	KW/CM3
DP(BEFORE)	=	-.40	%
DP(AFTER)	=	.06	%

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Fig. 4.17: Tabular summary of population densities and their rates of change (and effective time constants), electrical and optical parameters.

TIME T = 2.000E-07 SEC
PERCENTAGE CONTRIBUTION OF REACTION K TO DN(I)/DT, EXPRESSED (FOR EACH SPECIES)
AS A PERCENTAGE OF THE MAXIMUM RATE OCCURING FOR ALL REACTIONS INCLUDED

	K	RATE(K)	MAX %	RAD	E(-)	AR	AR*	KR	KR*	AR**	KR**	AR(+)	KR(+)
	1	7.386E+21	45.3			-26.564	45.323						
	2	4.892E+21	22.3					-22.339	16.765				
*	3	2.428E+20	1.5			-.873				1.490			
*	4	6.666E+19	.3					-.304			.228		
	5	1.630E+22	100.0				-100.000			100.000			
	6	2.918E+22	100.0						-100.000		100.000		
	7	1.671E+21	7.8		5.810	-6.008						7.794	
*	8	7.283E+20	4.1		2.533			-3.326					4.079
*	9	7.837E+20	4.8		2.725		-4.809					3.656	
	10	1.445E+21	8.1		5.027				-4.953				8.096
*	11	6.900E+19	.4		.240					-.423		.322	
*	12	2.403E+20	1.3		.836						-.824		1.346
*	13	4.689E+19	.3		-.163	.169	.288						
	14	3.638E+21	19.3		-12.651			16.610	12.466				
	15	2.875E+22	100.0		-100.000								
	16	1.932E+20	5.7			1.390							
	17	4.776E+21	88.7					43.611					
	18	2.143E+22	100.0		74.541	-77.087						100.000	
	19	6.124E+21	37.6			-22.025	37.578						
	20	4.416E+21	24.7		15.356			-20.162					24.732
	21	1.263E+21	5.8					-5.767	4.328				
	22	1.456E+22	100.0			-52.375						-67.943	
	23	2.024E+21	10.7					-9.243				-9.444	
	24	4.765E+21	26.7					-21.756					-26.688
	25	1.785E+22	100.0			-64.209							-100.000
	26	4.968E+21	27.8			17.868		-22.685				-23.179	27.828
	27	1.390E+22	100.0			100.000		-63.480					77.870
	28	1.889E+22	100.0			67.952		-86.272					
	29	3.400E+21	100.0			-12.227	-20.861						
	30	3.780E+20	7.0				-2.320	-1.726					
	31	3.323E+21	61.7					-15.173	-11.387				
	32	5.433E+21	100.0			-19.540			-18.619				
	33	5.385E+21	100.0			19.366		-24.587					
*	34	1.559E+20	3.4			.561							
*	35	1.559E+20	4.0										
	36	2.786E+21	60.0									-12.998	
	37	8.064E+21	42.7					36.822					
	38	8.064E+21	81.6										
	39	6.831E+21	38.3										-38.260
*	40	4.966E+20	2.6			1.786							
	41	4.966E+20	17.5										
	42	7.127E+21	32.5						-24.421				
	43	4.645E+21	100.0				-28.503						
	44	4.794E+21	29.4			17.241	-29.416	-21.889	16.428				
	45	2.621E+21	92.4			-9.425							
	46	2.428E+21	24.6					-11.088					
	47	3.890E+21	100.0			-13.988							
*	48	1.081E+20	3.8					-.494					
	49	3.062E+21	90.1			22.022		-13.980	10.492				
*	50	1.839E+16	.0		.000	.000							

* THIS REACTION CONTRIBUTES LESS THAN 5. % TO ALL SPECIES THROUGHOUT THE ENTIRE CALCULATION SO FAR

Fig. 4.18: (Partial) reproduction of tabular summary of reaction sensitivities.

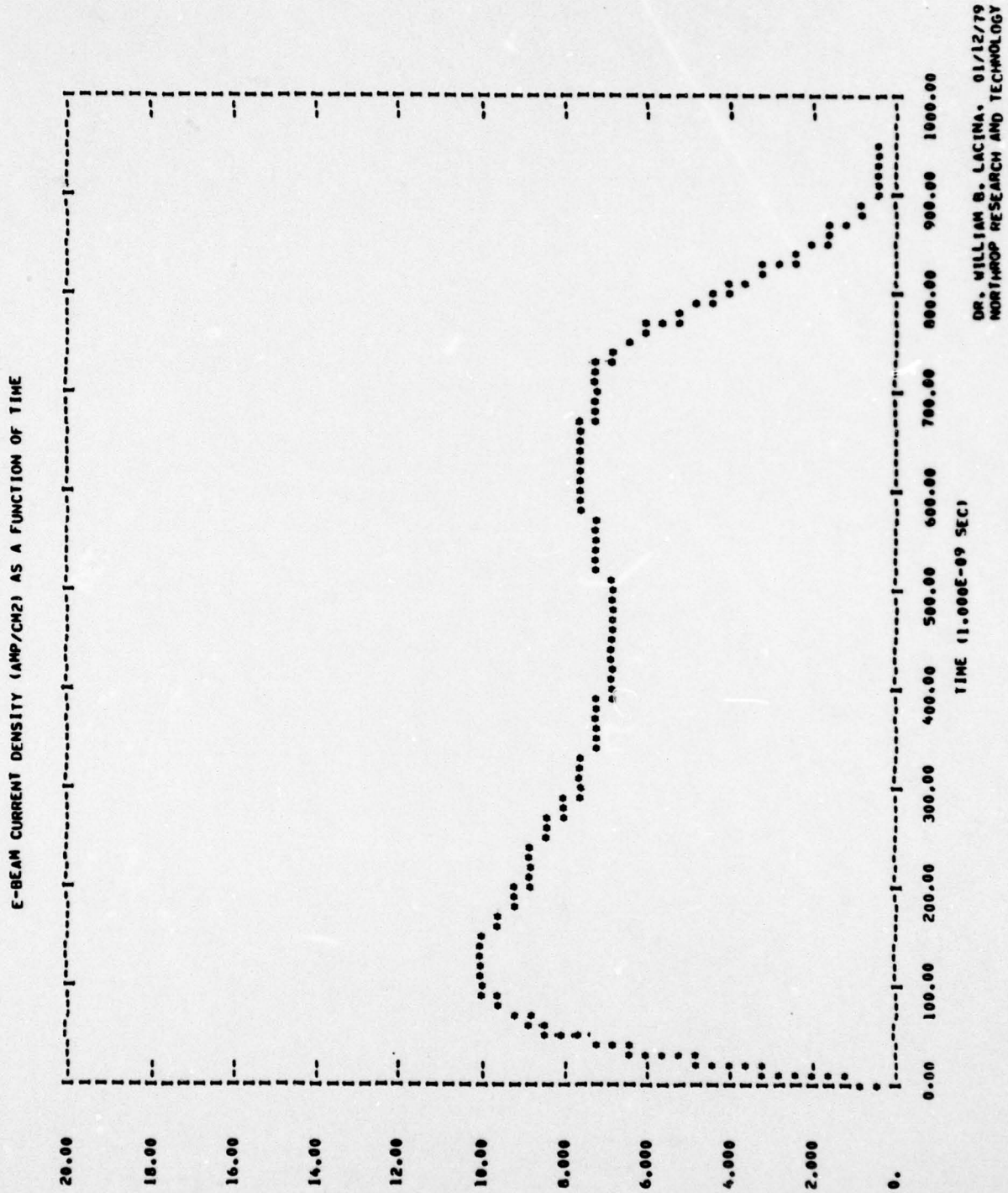

Fig. 4.19: Electron Beam current density as a function of time.

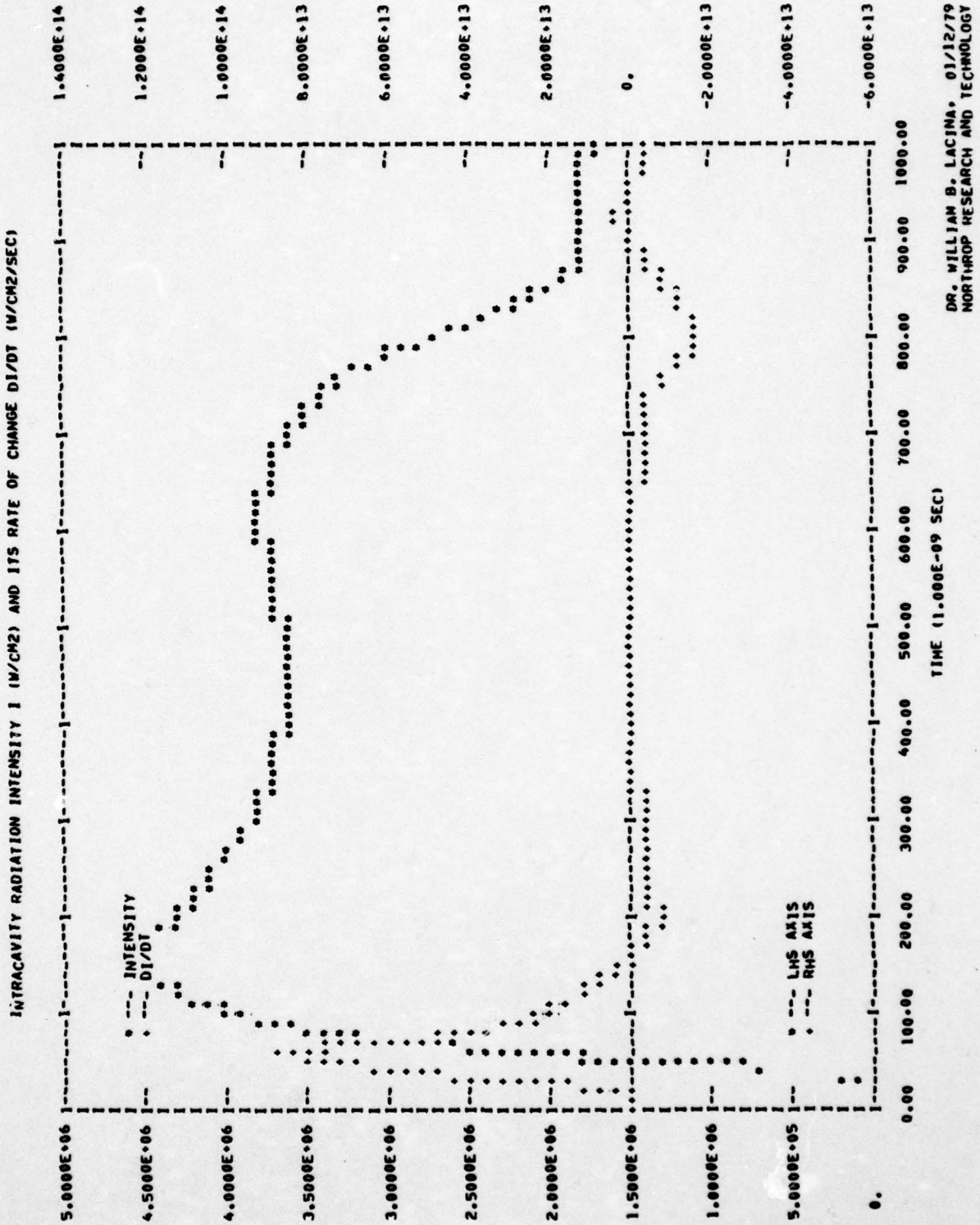

Fig. 4.20: Intracavity radiation intensity as a function of time.

SUMMARY OF ELECTRICAL AND OPTICAL PARAMETERS

TIME (1.00E-09 SEC)	JBEAM (A/CM2)	PBEAM (KW/CM3)	VOLTAGE (KV)	JSUS (A/CM2)	DISCH (KW/CM3)	OUTPUT (KW/CM3)	OPT EFF (%)
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10.00	2.15	32.92	3.80	.08	.03	-.00	-.00
20.00	4.05	57.09	.39	4.00	.16	.00	.00
30.00	5.69	82.19	2.38	1.49	.35	.41	.50
40.00	7.07	102.29	3.36	4.75	1.60	4.16	4.00
50.00	8.20	119.09	3.31	5.52	1.83	9.74	8.06
60.00	8.70	126.63	3.53	6.93	2.45	10.45	8.10
70.00	9.14	133.05	3.77	8.11	3.05	10.29	7.56
80.00	9.50	138.35	4.02	9.31	3.74	10.26	7.22
90.00	9.78	142.57	4.28	10.46	4.48	10.42	7.08
100.00	10.00	145.72	4.53	11.57	5.25	10.64	7.05
110.00	10.08	146.90	4.81	12.63	6.08	10.82	7.07
120.00	10.12	147.51	5.12	13.65	6.98	10.92	7.07
130.00	10.12	147.56	5.43	14.67	7.97	10.96	7.05
140.00	10.08	147.03	5.76	15.68	9.03	10.96	7.03
150.00	10.00	145.93	6.10	16.67	10.17	10.92	6.99
160.00	9.76	142.52	6.50	17.56	11.41	10.77	7.00
170.00	9.54	139.43	6.95	18.42	12.80	10.53	6.91
180.00	9.34	136.64	7.41	19.35	14.34	10.28	6.81
190.00	9.16	134.14	7.87	20.31	15.99	10.07	6.70
200.00	9.00	131.92	8.31	21.26	17.67	9.88	6.61
210.00	8.92	130.92	8.72	22.23	19.38	9.75	6.49
220.00	8.84	129.71	9.07	23.22	21.06	9.69	6.42
230.00	8.74	128.32	9.41	24.09	22.67	9.64	6.38
240.00	8.62	126.76	9.75	24.93	24.31	9.57	6.34
250.00	8.50	125.02	10.10	25.73	26.00	9.49	6.29
260.00	8.31	122.28	10.49	26.47	27.76	9.38	6.25
270.00	8.13	119.80	10.90	27.16	29.62	9.23	6.18
280.00	7.97	117.54	11.33	27.92	31.63	9.09	6.09
290.00	7.83	115.51	11.73	28.72	33.68	8.96	6.01
300.00	7.70	113.69	12.09	29.50	35.65	8.88	5.94
310.00	7.62	112.57	12.40	30.28	37.54	8.82	5.88
320.00	7.54	111.43	12.66	31.05	39.30	8.80	5.84
330.00	7.46	110.28	12.88	31.74	40.88	8.79	5.82
340.00	7.38	109.13	13.09	32.36	42.37	8.78	5.79
350.00	7.30	107.98	13.30	32.99	43.86	8.75	5.76
360.00	7.20	106.59	13.50	33.55	45.30	8.72	5.74
370.00	7.12	105.32	13.71	34.09	46.75	8.68	5.71
380.00	7.04	104.17	13.91	34.66	48.22	8.64	5.67
390.00	6.96	103.13	14.09	35.22	49.61	8.61	5.64
400.00	6.90	102.19	14.23	35.76	50.90	8.59	5.61
410.00	6.83	101.14	14.36	36.26	52.07	8.57	5.60
420.00	6.77	100.32	14.47	36.73	53.15	8.55	5.57
430.00	6.73	99.73	14.56	37.21	54.17	8.53	5.54
440.00	6.71	99.37	14.61	37.70	55.07	8.53	5.52
450.00	6.70	99.24	14.60	38.20	55.78	8.54	5.51
460.00	6.73	99.69	14.54	38.70	56.26	8.56	5.49
470.00	6.77	100.18	14.42	39.16	56.49	8.61	5.49
480.00	6.81	100.73	14.28	39.55	56.48	8.65	5.50
490.00	6.85	101.33	14.13	39.88	56.36	8.69	5.51
500.00	6.90	102.00	13.98	40.19	56.20	8.72	5.51

Fig. 4.21: Tabular summary of miscellaneous electrical and optical parameters as a function of time (voltages, current, power densities).

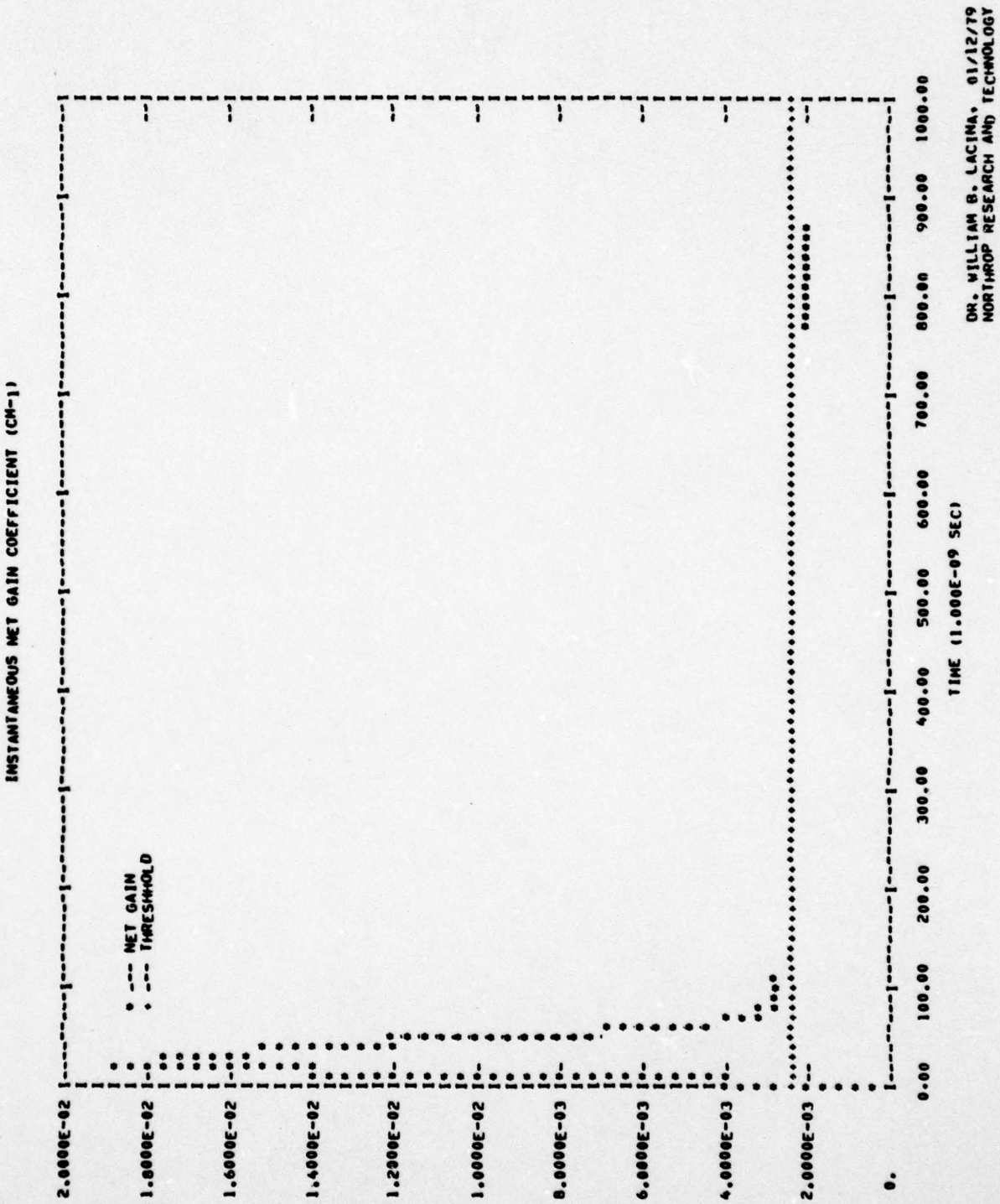

Fig. 4.22: Instantaneous net gain coefficient, relative to threshold, as a function of time.

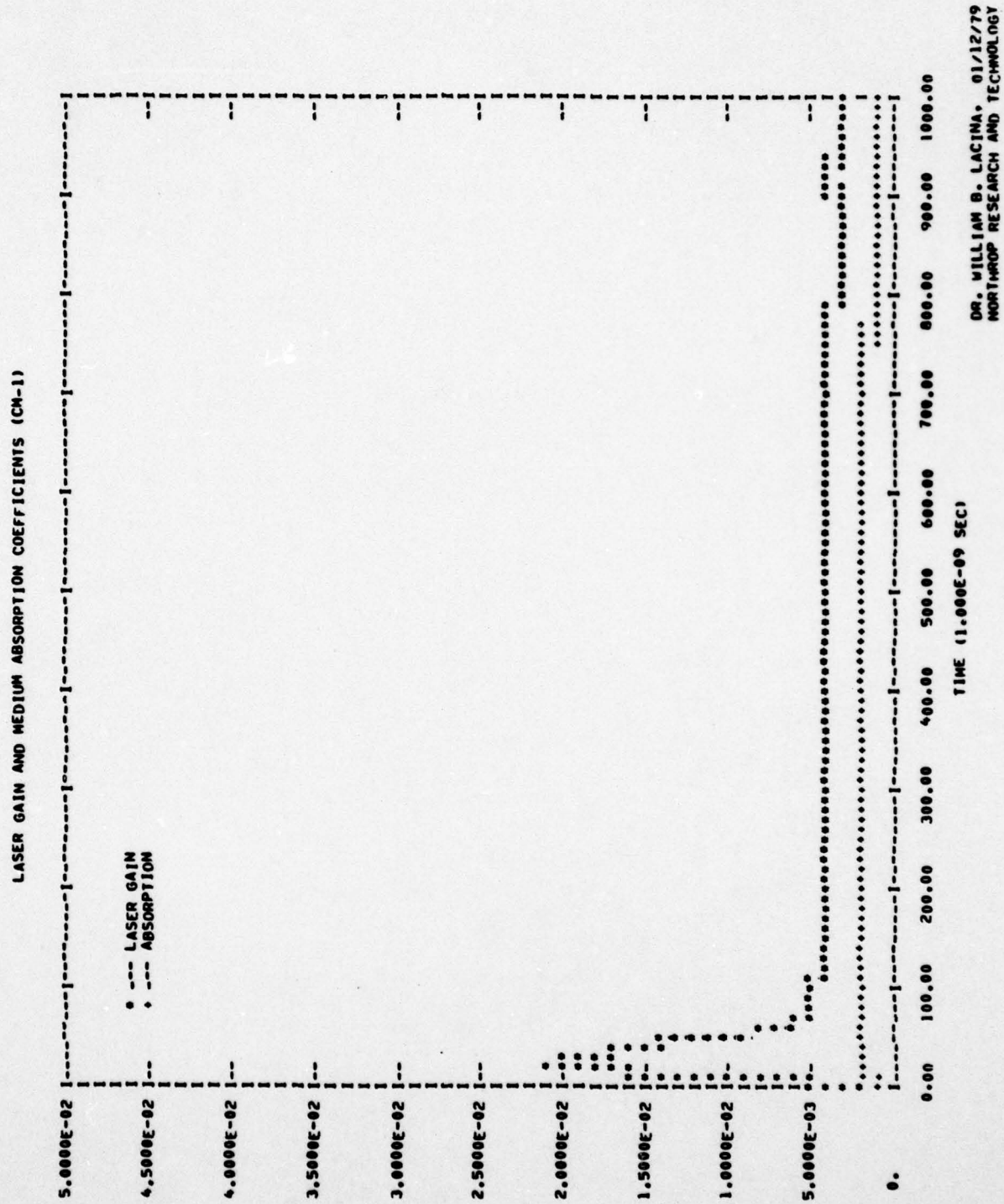

Fig. 4.23: Medium gain and absorption coefficients.

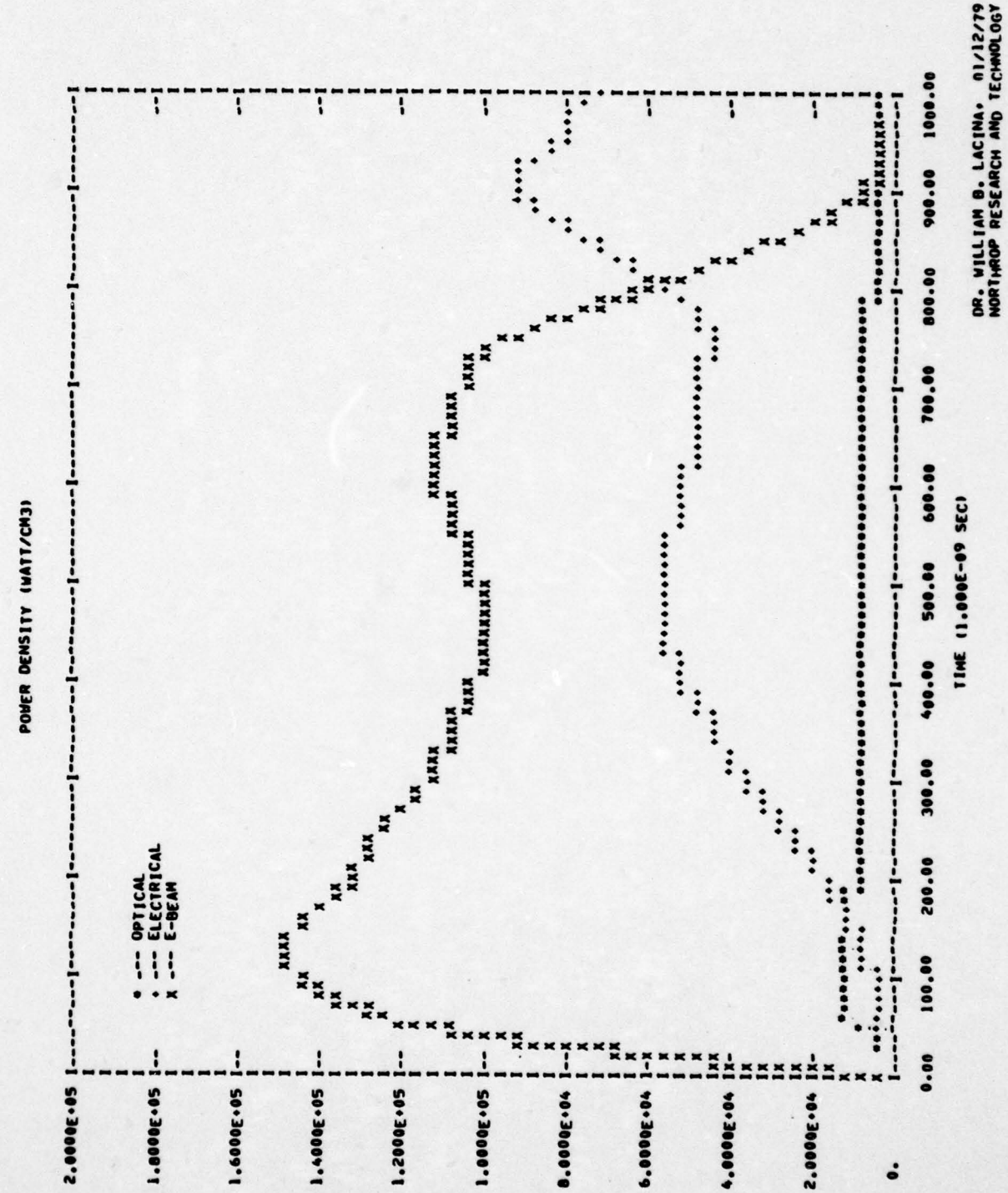

Fig. 4.24: Electrical and optical power densities.

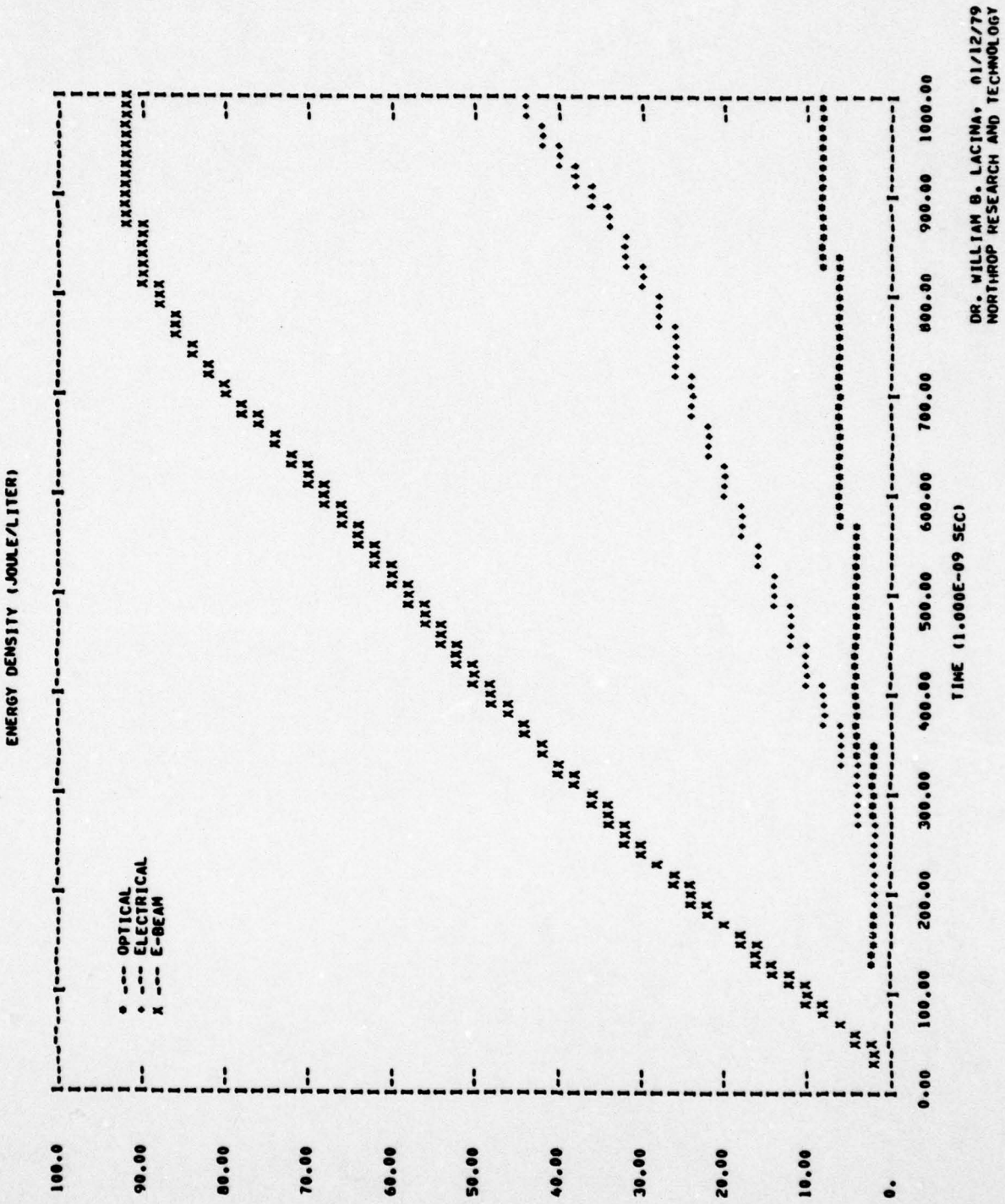

Fig. 4.25: Total (integrated) electrical and optical energy densities as a function of time.

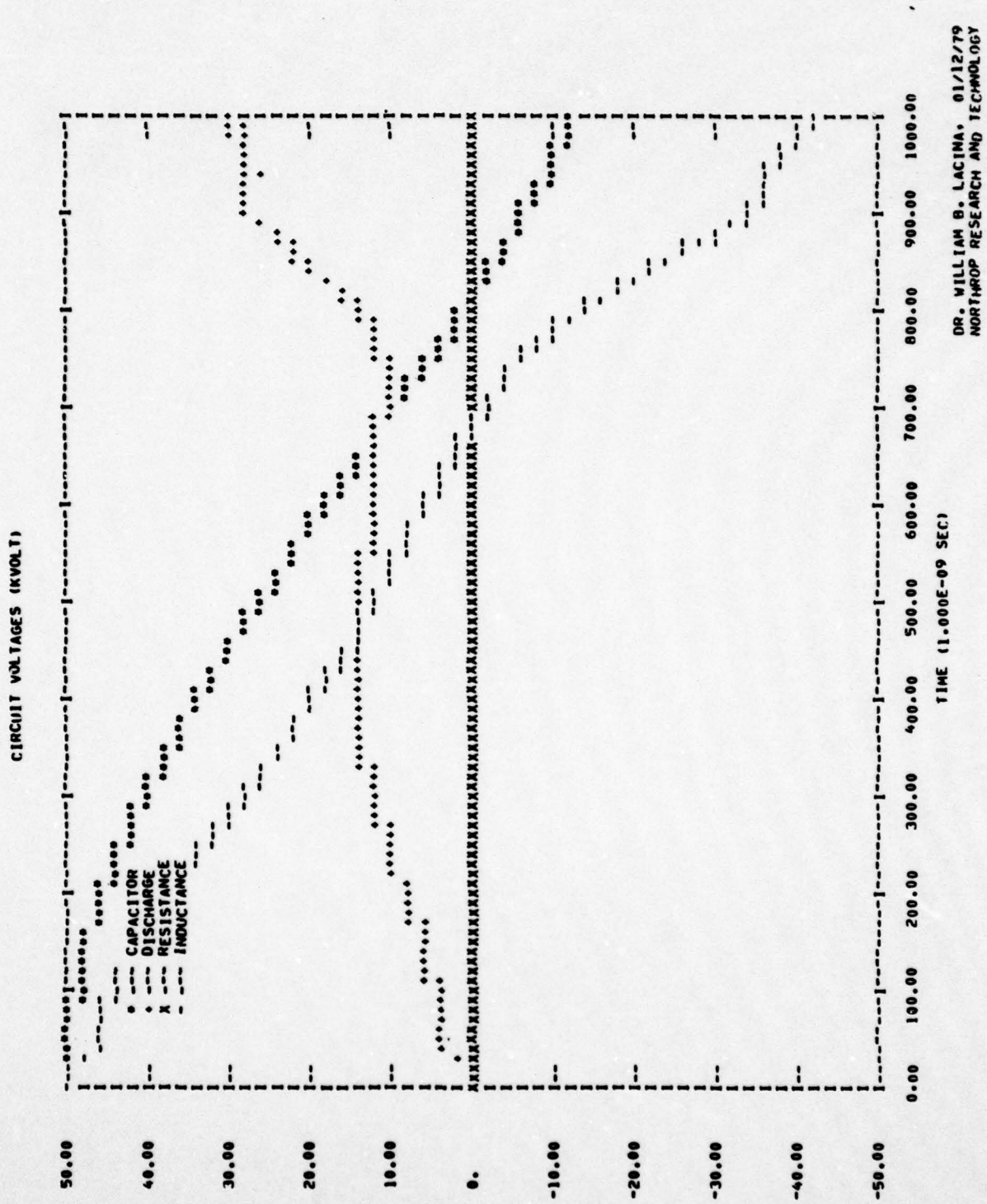

Fig. 4.26: Circuit voltages.

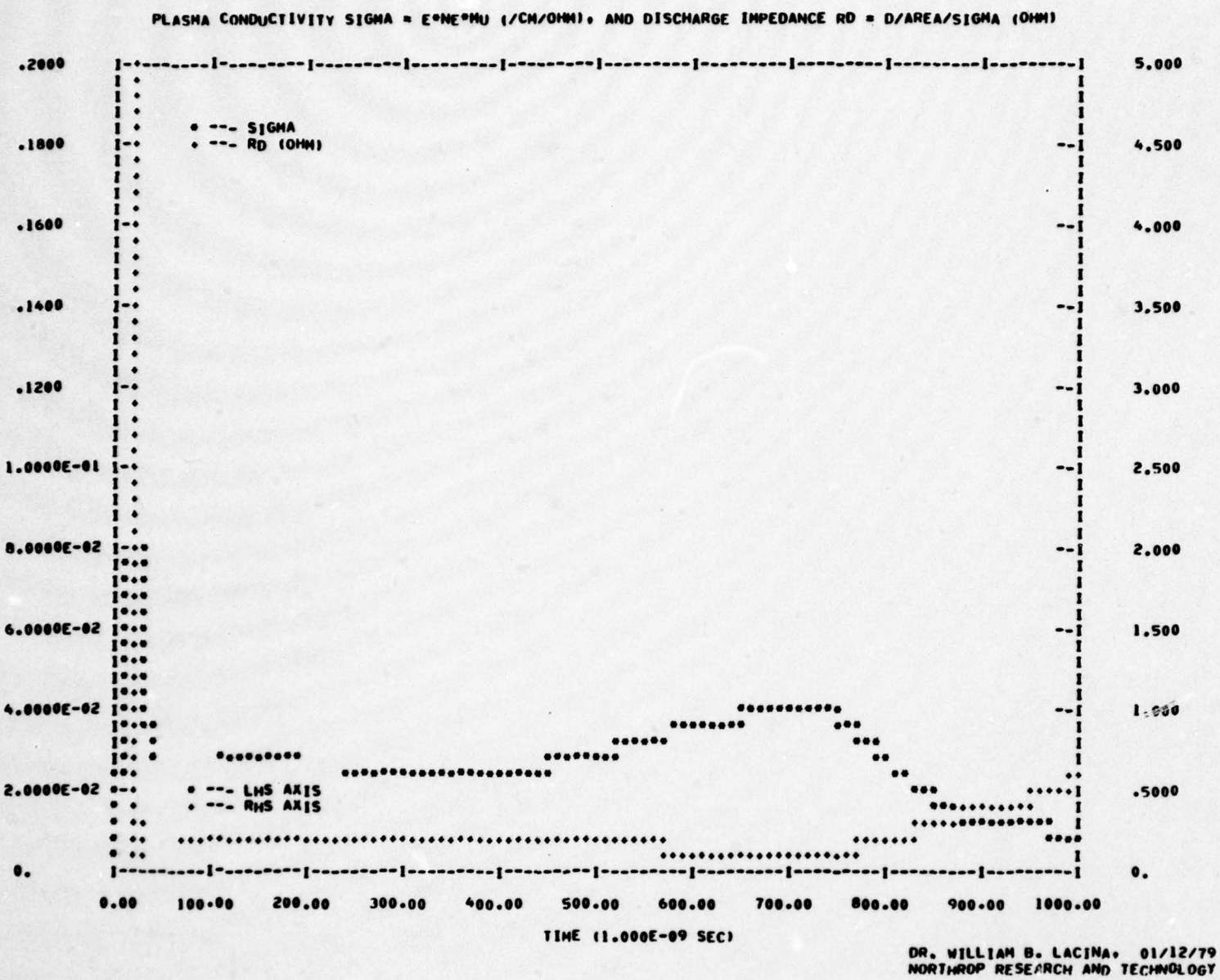

Fig. 4.27: Plasma conductivity and impedance.

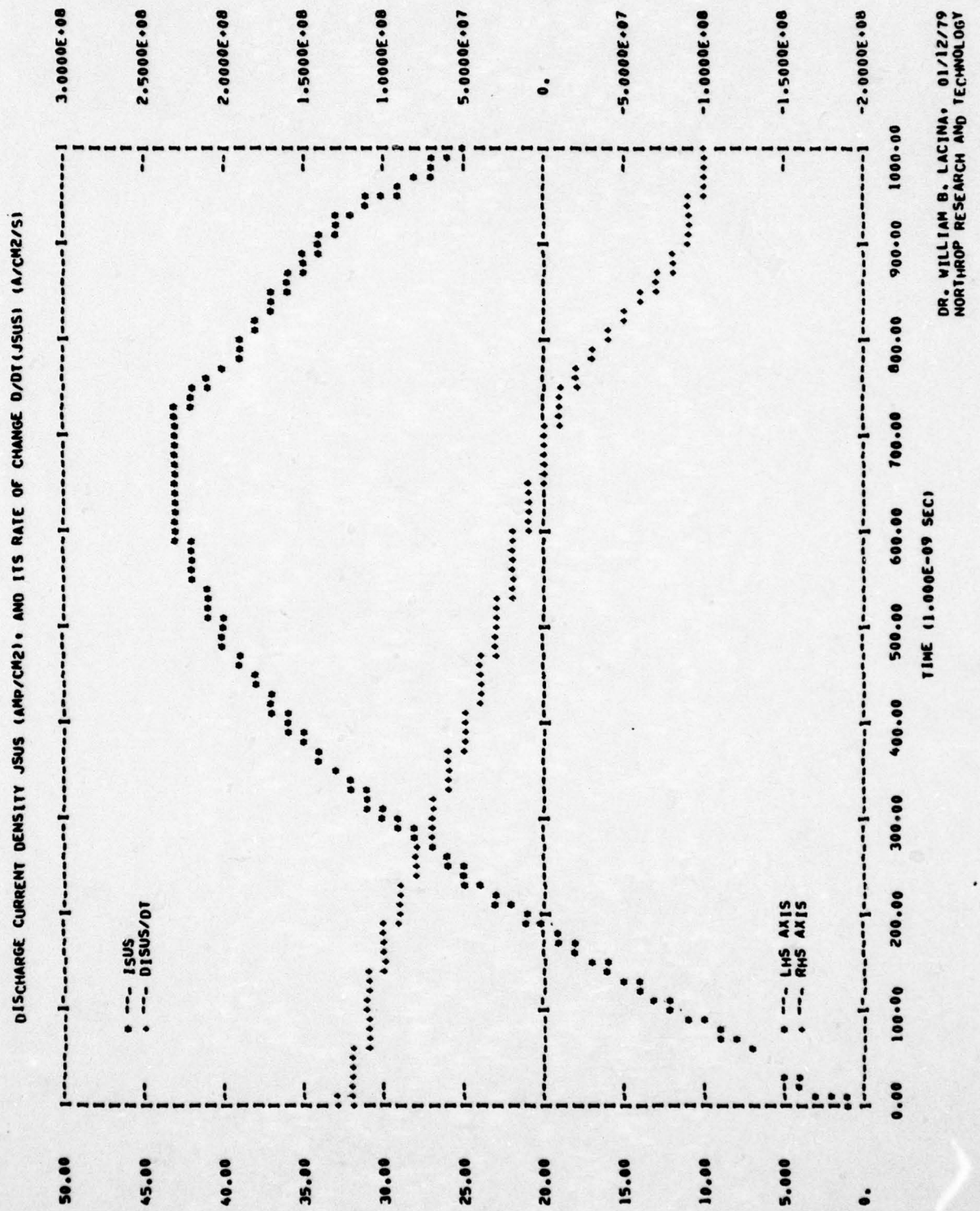

Fig. 4.28: Discharge current density.

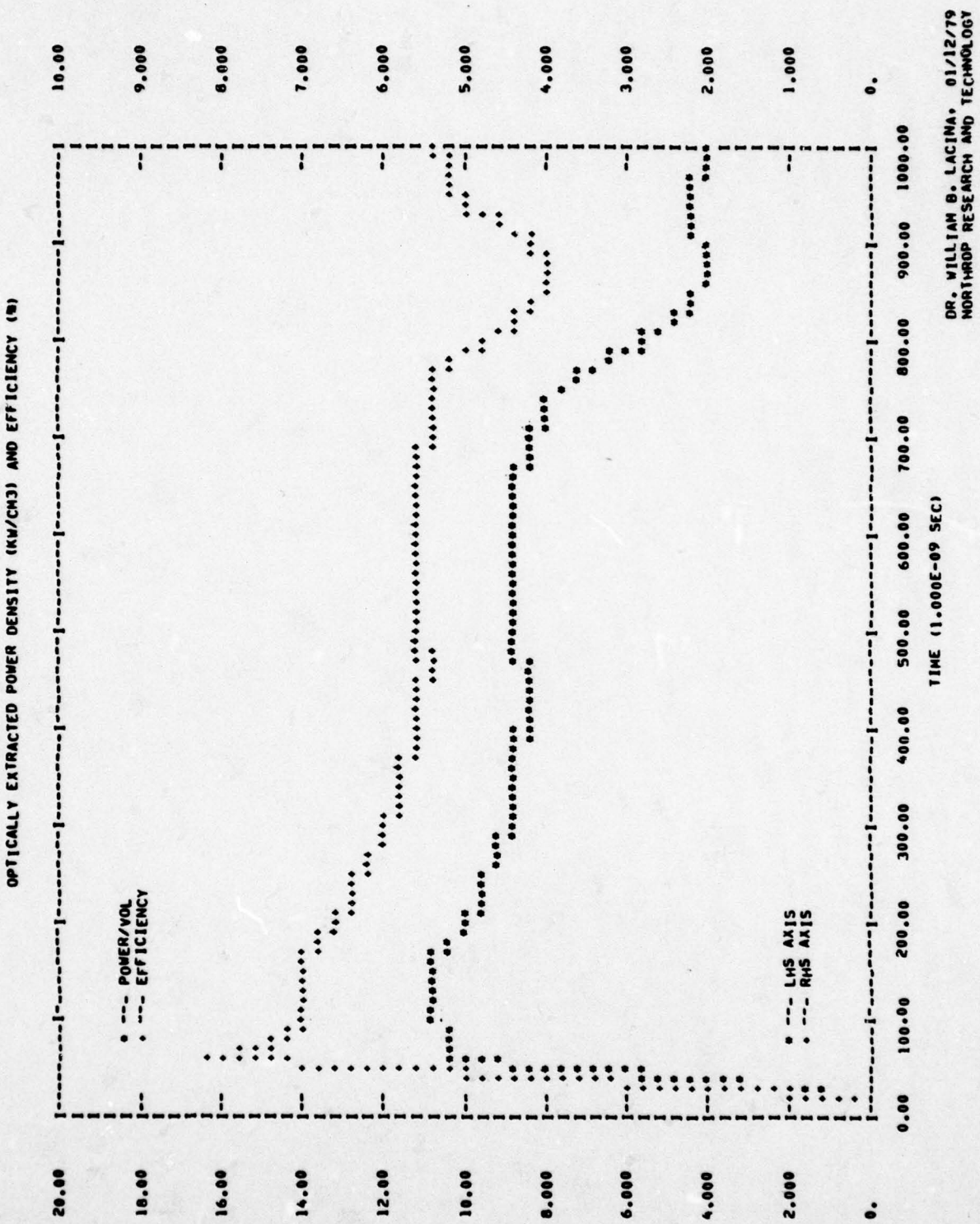

Fig. 4.29: Optically extracted power density, efficiency.

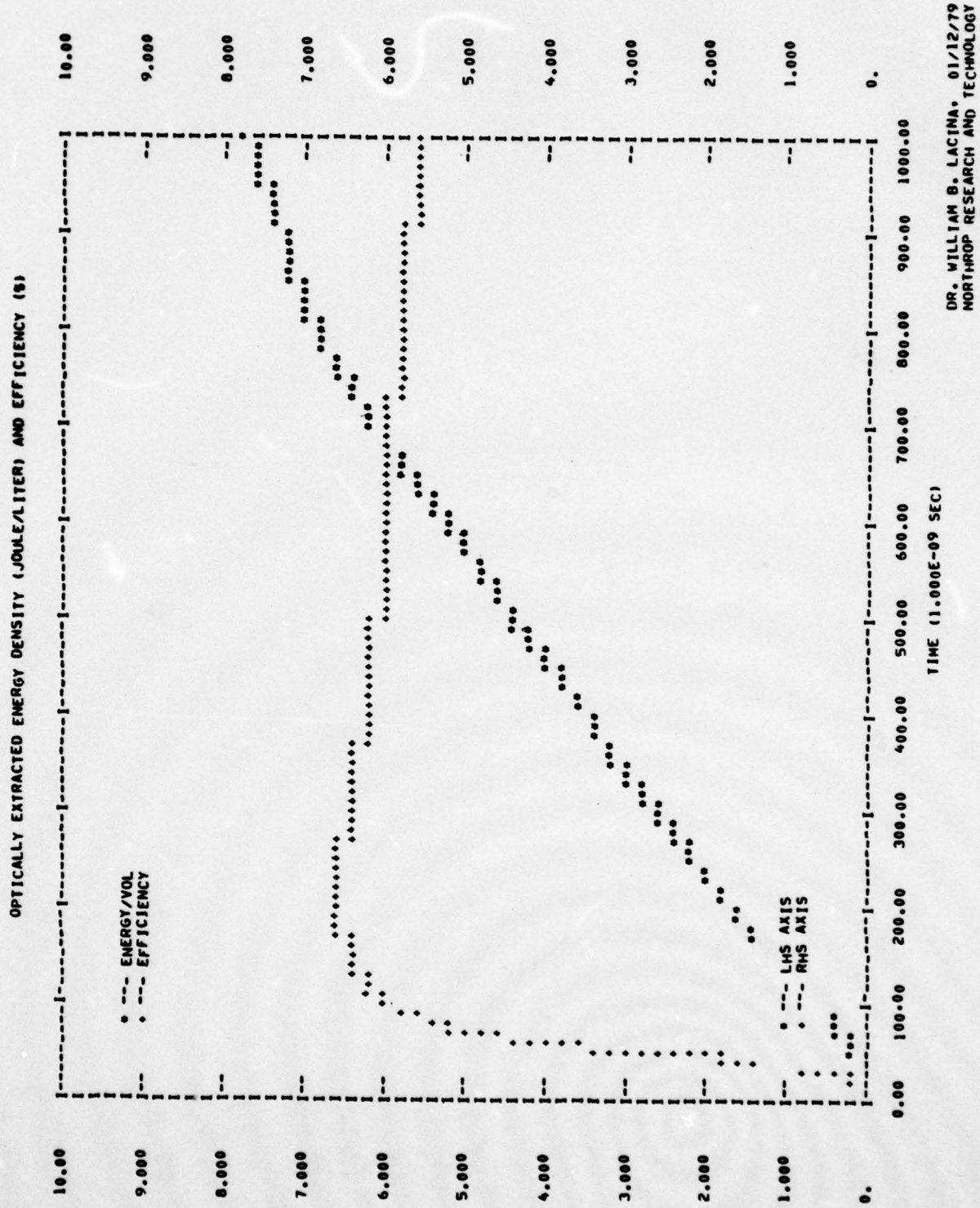

Fig. 4.30: Optically extracted energy density and efficiency.

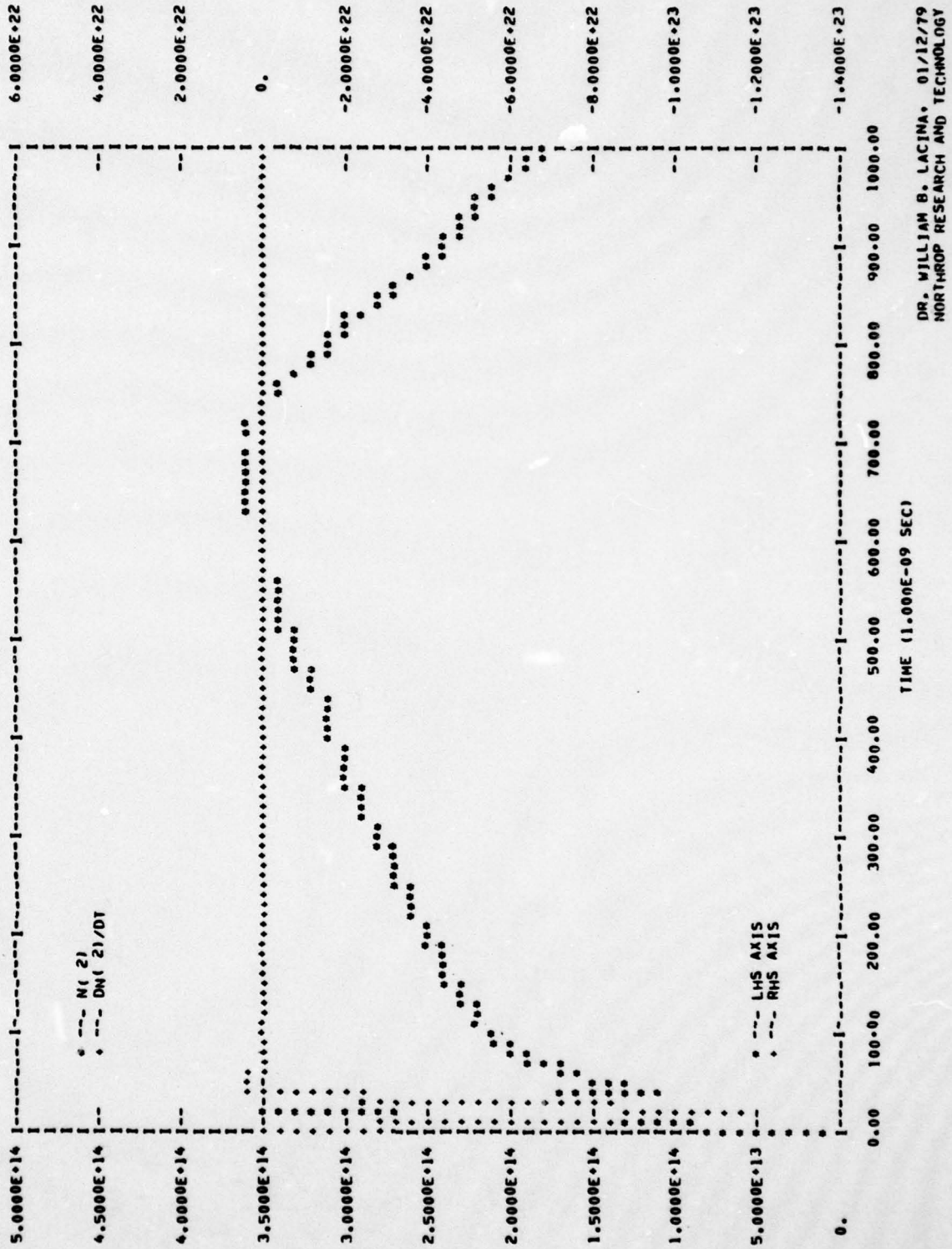

Fig. 4.31: Population density and rate of change for e^-.

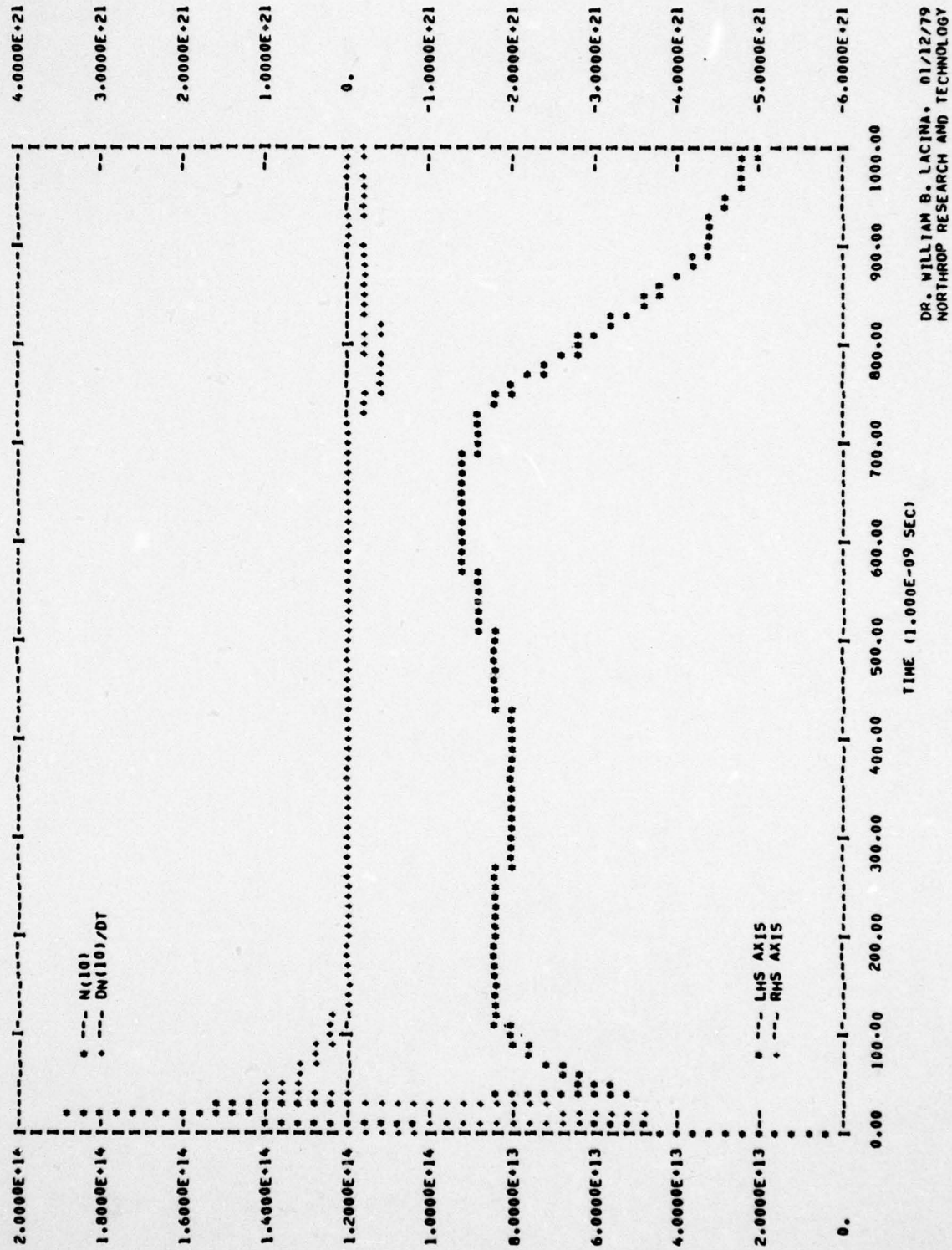

Fig. 4.32: Population density and rate of change for Kr^+.

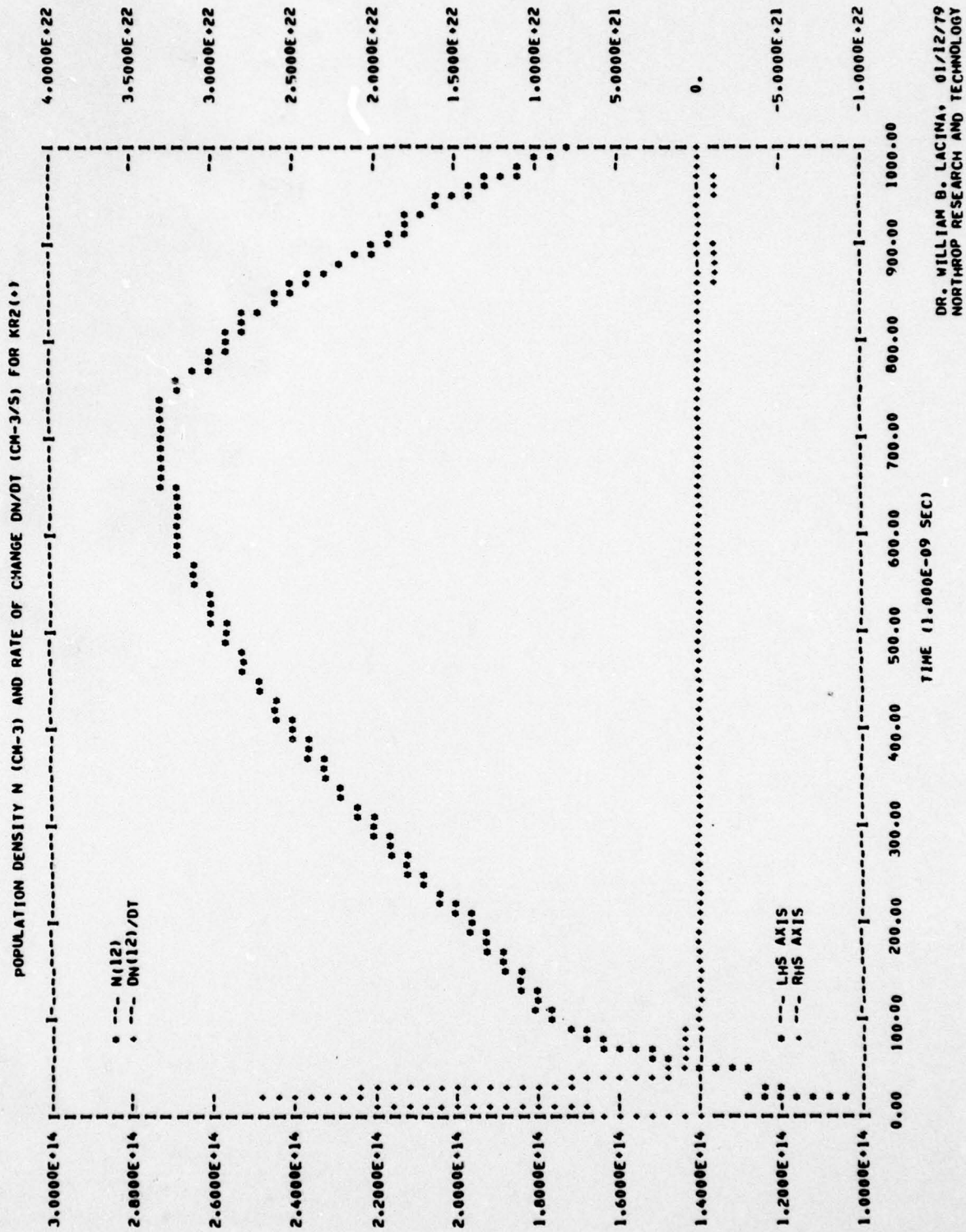

Fig. 4.33: Population density and rate of change for Kr_2^+.

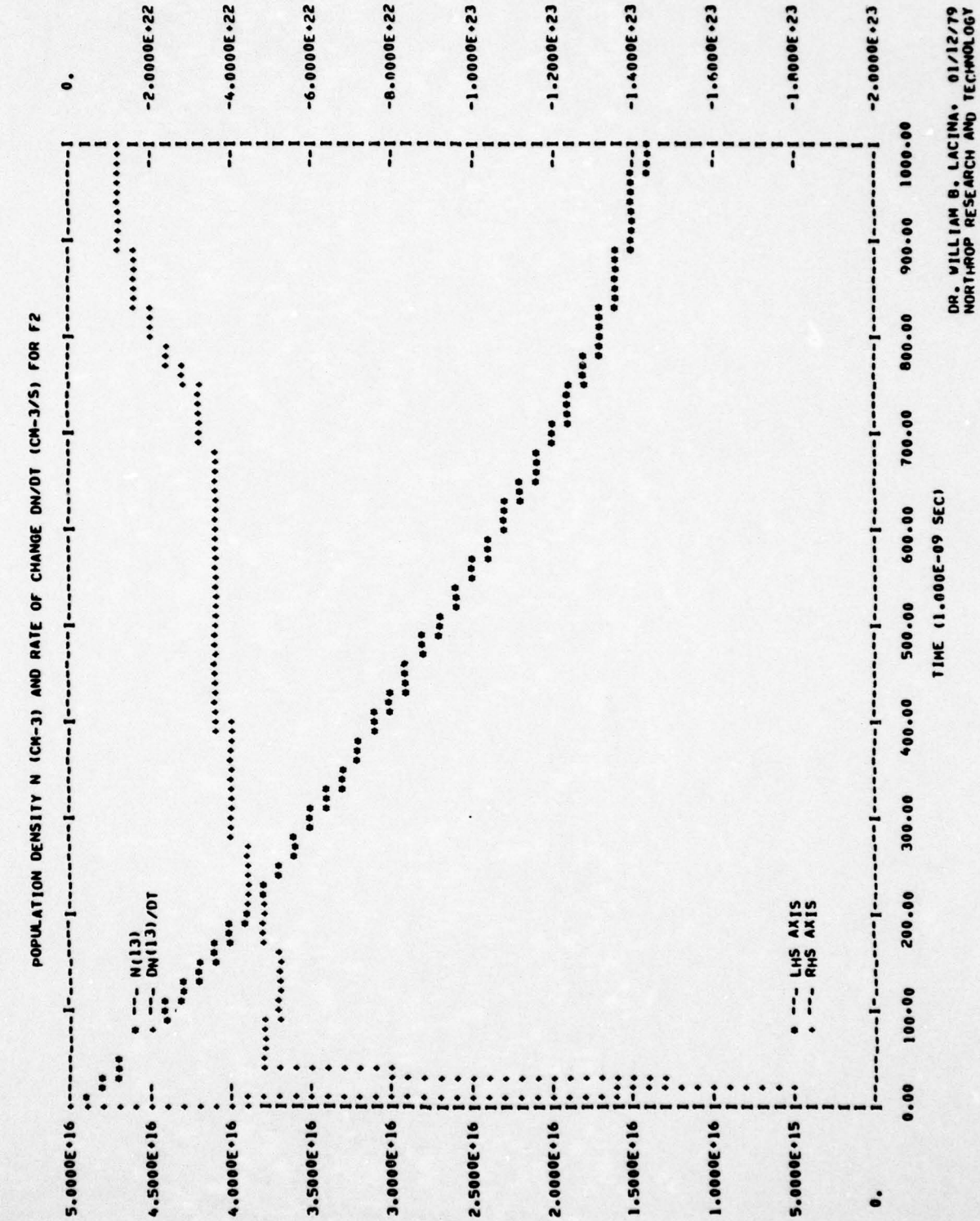

Fig. 4.34: Population density and rate of change for F_2.

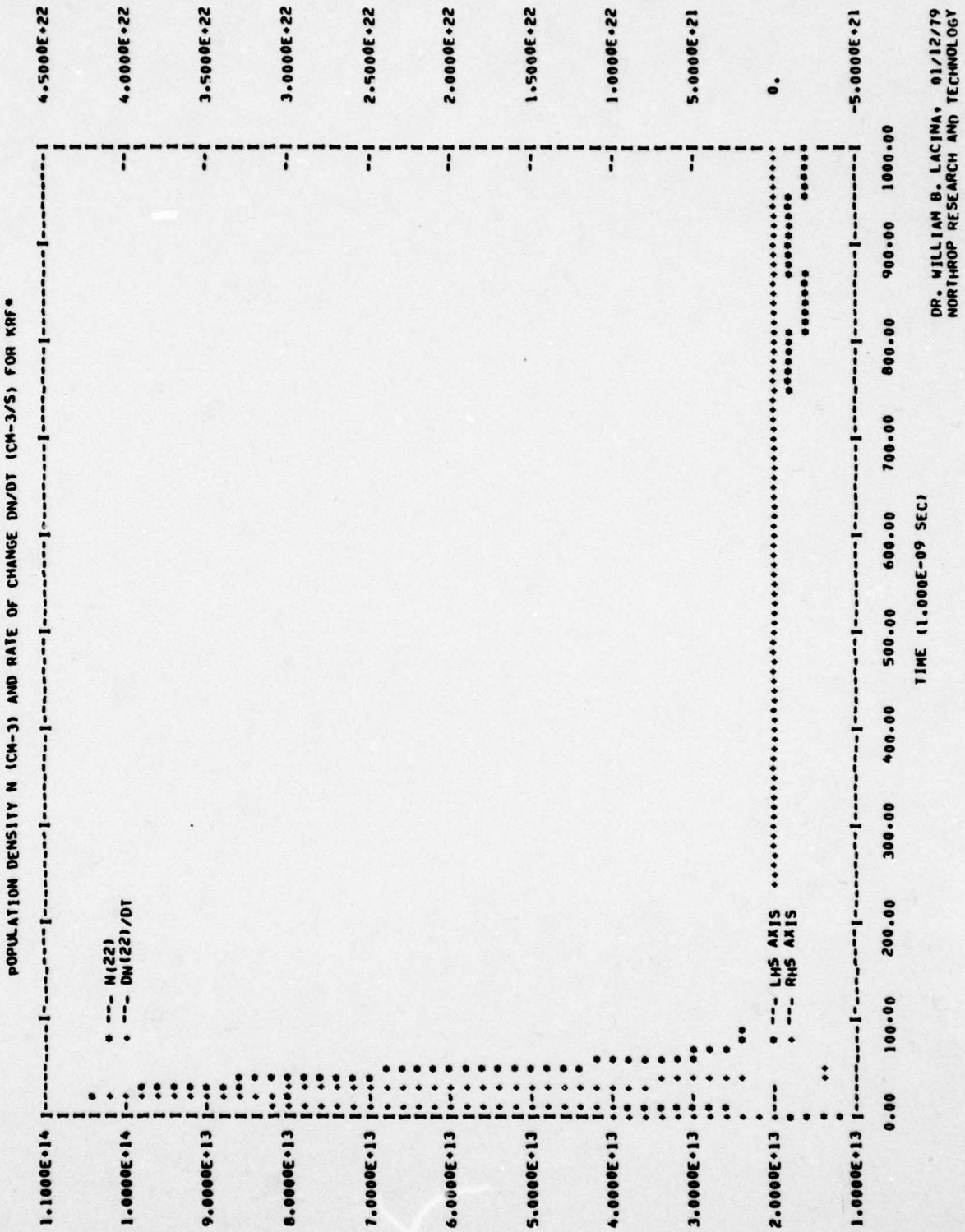

Fig. 4.35: Population density and rate of change for KrF*.

4.3 Error Diagnostic Assistance

Although it is not possible to anticipate all possible forms of incorrect usage, program LASER has been designed to provide limited diagnostic assistance upon recognition of certain (potential) error conditions. The search for errors occurs in processing an input reaction queue for subroutine synthesis, and at the time of data input for execution of the analysis.

The DATA BLOCK 1 shown in Fig. 4.36 violates several of the conventions described in Sec. 3.2. Assume that program LASER has been dimensioned NMAX = 30, KMAX = 16, and NKMAX = 8 (for purposes of illustration), and that DATA BLOCK 1 is submitted for a program synthesis. Even if the reaction syntax contained no intrinsic defects, its species content and total length would exceed the dimension capacity specified for LASER.

The reaction summary generated in an attempt to process the DATA BLOCK 1 of Fig. 4.36 contains numerous informative and diagnostic comments, as shown in Fig. 4.37. For defective reactions, there is no FORTRAN translation: the reaction is ignored (and unnumbered in Fig. 4.37), and processing continues. The data file generated (unit 4) contains, in addition to the rate constant data, a logical parameter (written in the second record) whose value is .TRUE. or .FALSE. depending upon whether or not errors were encountered. A later attempt to execute an incomplete analysis from which reactions were rejected can be prohibited by specifying FATAL(1) = .TRUE.

Return now to the KrF program, synthesized from the reaction scheme of Fig. 4.1 to produce the subroutines illustrated in Fig. 4.2 - 4.4. For

the purpose of illustrating execution error diagnostics, suppose that the original kinetic scheme of Fig. 4.1 had contained some (unimportant) error, such as the rejection of a duplicate reaction. (Thus, for all practical purposes, files KRFBCD and KRFLASER are completely satisfactory, although KRFDATA will contain a record of the fact that a defect had been encountered during synthesis.) Suppose, furthermore, that the dimension declarators in LASER have been changed since the original creation of the KrF files, and that execution of the analysis is attempted with the input DATA BLOCK 4 shown in Fig. 4.38. Note that no specification of the vector FATAL(I) appears in the data group $CONTROL ... $ to override the default initialization .FALSE. Note further that Fig. 4.38 differs from Fig. 4.7 in that now, there are rate constant modifications specified by $RATES ... $ entry, and a new species "XXX" has been initialized. (Most of the other parameters are numerically different, but that is not relevant for the point to be illustrated here.) Fig. 4.39 is the tabular summary of the reaction scheme and its modified rate constants; note that some of the attempted modifications were illegal and were rejected. Fig. 4.40 is a summary of error diagnostics encountered in the attempt to execute the analysis.

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                              (DATE: 02/02/79)

CARD            1         2         3         4         5         6         7         8
 NO.   12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------

  1 ....TEST CASE CONTAINING ERRORS
  2 ....AR2F* + F2 ,, AR + KR + F + F2
  3 .... 1.00 E-09                 SRI REPORT, DEC. 1976.
  4 ....F2 + AR2F* ,,  F+F2  + KR  +AR
  5 .... 1.00 E-09                 SRI REPORT, DEC. 1976.
  6 ....XY + E ,, XY** + E
  7 ....                           AN ANONYMOUS SOURCE
  8 ....XY + E ,, XY* + E
  9 .... 1.00 E-08 1.40 E-09       REFERENCE: PHYS. REV. 12, 22 (1728)
 10 ....AR + E ,, AR* + E
 11 ....
 12 ....AR + E ,, AR(+) + E + E
 13 ....                           RAPP, ENGLANDER-GOLDEN, J. CHEM PHYS. 43,1464 (65)
 14 ....KR + E ,, KR* + E
 15 ....                           SCHAPER, SCHEIBNER, BEITR. AUS PLASMA PHYS. 9, 45
 16 ....KR + E ,, KR(+) + E + E
 17 ....
 18 ....XY + E ,, XY(+) + E
 19 ....                           DECREED BY VOTE OF THE LEGISLATURE
 20 ....XY + E ,, XY* + E
 21 ....         1.        1.      FROM A USUALLY UNRELIABLE SOURCE
 22 ....AR* + E ,, AR(+) + E + E
 23 ....
 24 ....KR* + E ,, KR(+) + E + E
 25 ....
 26 ....   AR** +E-  ,, AR(+) + 2E-
 27 ....
 28 ....KR** + E- ,, KR(+) + E- + E-
 29 ....
 30 ....XY + E ,, XY+  + E + E
 31 ....
 32 ....XY* + E ,, XY + E
 33 ....         1.        1.
 34 ....KR2(+) + E ,, KR + KR*
 35 ....
 36 ....AR2(+) + E ,, AR + AR*
 37 ....
 38 ....F2 + E ,, F + F-
 39 ....
 40 ....AR(+) + E ,, AR(2+) + E + E
-------------------------------------------------------------------------------------

       12345678901234567890123456789012345678901234567890123456789012345678901234567890
                1         2         3         4         5         6         7         8
```

Fig. 4.36: Defective DATA BLOCK 1.

```
                    SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
                                (DATE: 02/02/79)

CARD              1         2         3         4         5         6         7         8
 NO.    12345678901234567890123456789012345678901234567890123456789012345678901234567890
-----------------------------------------------------------------------------------------

 41 ....          1.        1.
 42 ....AR(+) + E ↵ AR(++) + E + E
 43 ....          1.        1.
 44 ....AR + KR* ↵ KR + AR*
 45 ....          1.
 46 ....A + B + XYZ --> AX + BY + Z
 47 .... 4.50 E-10 5.00 E-09      KNOWN SINCE ANTIQUITY
 48 ....AR(+) + KR ↵ AR + KR(+)
 49 .... 3.00 E-11
 50 ....KR2* + M ↵ KR + KR
 51 ....          1.
 52 ....KR2* + M ↵ KR + KR + M
 53 ....          1.        1.
 54 ....XY + HE- ↵ XY(+) + HE- + HE-
 55 ....          1.        1.
 56 ....AR + HE- ↵ AR(+) + HE- + E-
 57 ....          1.        1.
 58 ....A + XY + B + C + AR + KR ↵ A* + XY(+) + E + B + C + AR + KR*
 59 ....          1.        1.
 60 ....KR* + AR ↵ AR* + KR
 61 ....          1.        2.
 62 ....KRF* + RAD ↵ KR + F + RAD
 63 ....          1.        1.      STIMULATED EMISSION PROCESS.
 64 ....XY* ↵ X + Y* + RAD
 65 ....          1.        1.
 66 ....F- + RAD ↵ F + E
 67 .... 5.40 E-18                 A. MANDL, PHYS. REV. A3, 251 (1971)
 68 ....KRF* ↵ KR + F + HNU
 69 .... 1.10 E 08                 BURNHAM AND SEARLES
 70 ....XY* ↵ XY
 71 ....          1.        1.
 72 ....           AB  + E ↵                  A + B                    + E
 73 ....          1.        1.
-----------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.36: Defective DATA BLOCK 1 (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
1	AR2F* + F2 → AR + KR + F + F2	1.0000E-09		SRI REPORT, DEC. 1976. REVERSE REACTION IS IGNORED -- KR = 0.
	F2 + AR2F* → F + F2 + KR + AR	1.0000E-09		SRI REPORT, DEC. 1976. REACTION IGNORED -- SAME AS NUMBER 1. REVERSE REACTION IS IGNORED -- KR = 0.
2	XY + E → XY** + E	(COMPUTED)	(COMPUTED)	AN ANONYMOUS SOURCE WARNING -- NO E- CROSS SECTION DATA WAS FOUND. FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
3	XY + E → XY* + E	1.0000E-08	1.4000E-09	REFERENCE* PHYS. REV. 12, 22 (1728)
4	AR + E → AR* + E	(COMPUTED)	(COMPUTED)	FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
5	AR + E → AR(+) + E + E	(COMPUTED)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
6	KR + E → KR* + E	(COMPUTED)	(COMPUTED)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45 FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS REVERSE RATE IS OBTAINED FROM E- KINETICS ANALYSIS
7	KR + E → KR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	XY + E → XY(+) + E			DECREED BY VOTE OF THE LEGISLATURE REACTION REJECTED -- CHARGE CONSERVATION VIOLATED.
	XY + E → XY* + E	1.0000E+00	1.0000E+00	FROM A USUALLY UNRELIABLE SOURCE REACTION IGNORED -- SAME AS NUMBER 3.
8	AR* + E → AR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
9	KR* + E → KR(+) + E + E	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 02/02/79

Fig. 4.37: Summary of defective reaction scheme.

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
	AR** + E- → AR(+) + 2E-			REACTION REJECTED -- CHARGE CONSERVATION VIOLATED. REVERSE REACTION IS IGNORED -- KR = 0.
10	KR** + E- → KR(+) + E- + E-	(COMPUTED)		FORWARD RATE IS OBTAINED FROM E- KINETICS ANALYSIS E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	XY + E → XY +			BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
	XY* + E → XY + E	1.0000E+00	1.0000E+00	REACTION IGNORED -- REVERSE OF NO. 3.
	KR2(+) + E → KR + KR*			REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	AR2(+) + E → AR + AR*			REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	F2 + E → F + F-			REACTION REJECTED -- NO MORE THAN 8 REACTIONS ARE ALLOWED FOR THE COUPLED E- KINETICS ANALYSIS. REVERSE REACTION IS IGNORED -- KR = 0.
	AR(+) + E → AR(2+) + E + E	1.0000E+00	1.0000E+00	REACTION REJECTED -- CHARGE CONSERVATION VIOLATED. E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
11	AR(+) + E → AR(++) + E + E	1.0000E+00	1.0000E+00	E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
12	AR + KR* → KR + AR*	1.0000E+00	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	A + B + XYZ-->AX + BY + Z			KNOWN SINCE ANTIQUITY BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
13	AR(+) + KR → AR + KR(+)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	KR2* + M → KR + KR	1.0000E+00		IMPROPER BUFFER GAS SPECIFICATION. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED. REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
14	KR2* + M → KR + KR + M	1.0000E+00	1.0000E+00	

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 02/02/79

Fig. 4.37: Summary of defective reaction scheme (cont'd).

SUMMARY OF INPUT: REACTIONS AND RATE CONSTANTS (SEC-1, CM3/SEC, CM6/SEC, ..., OR CM2) WITH REFERENCES

(IF A RATE CONSTANT KF OR KR FOR A BINARY ELECTRON COLLISION IS NOT EXPLICITLY SPECIFIED, IT WILL BE COMPUTED SELF CONSISTENTLY AS A FUNCTION OF E/N, GAS COMPOSITION, AND EXCITED LEVEL DENSITIES FROM A COUPLED ELECTRON ANALYSIS.)

I	REACTION(I) (IGNORED REACTIONS ARE NOT NUMBERED)	RATE CONSTANTS KF(I)	KR(I)	RATE REFERENCES AND/OR COMMENTS
	XY + HE- → XY(+) + HE- + HE-	1.0000E+00	1.0000E+00	IMPROPER HIGH ENERGY ELECTRON TERMS. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED. REACTION REJECTED -- CHARGE CONSERVATION VIOLATED.
15	AR + HE- → AR(+) + HE- + E-	1.0000E+00	1.0000E+00	E- CREATION ASSUMED TO BE OVER ENERGY DISTRIBUTION
	A + XY + B + C + AR + KR			> 5 SPECIES ON LHS OR RHS NOT PERMITTED. BAD SYNTAX -- UNRECOGNIZABLE REACTION IS IGNORED.
	KR* + AR → AR* + KR	1.0000E+00	2.0000E+00	REACTION IGNORED -- SAME AS NUMBER 12.
16	KRF* + RAD → KR + F + RAD	1.0000E+00	1.0000E+00	STIMULATED EMISSION PROCESS.
	XY* → X + Y* + RAD	1.0000E+00	1.0000E+00	THIS RADIATIVE PROCESS NOT ALLOWED. MORE THAN 16 REACTIONS ARE IGNORED.
	F- + RAD → F + E	5.4000E-18		A. MANDL, PHYS. REV. A3, 251 (1971) MORE THAN 16 REACTIONS ARE IGNORED. E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY REVERSE REACTION IS IGNORED -- KR = 0.
	KRF* → KR + F + HNU	1.1000E+08		BURNHAM AND SEARLES MORE THAN 16 REACTIONS ARE IGNORED. REVERSE REACTION IS IGNORED -- KR = 0. NO REVERSE REACTION ALLOWED FOR RADIATIVE DECAY.
	XY* → XY	1.0000E+00	1.0000E+00	MORE THAN 16 REACTIONS ARE IGNORED.
	AB + E → A + B + E	1.0000E+00	1.0000E+00	REACTION IS IGNORED -- MORE THAN 20 DIFFERENT GAS SPECIES ARE NOT PERMITTED WITH PRESENT DIMENSION. MORE THAN 16 REACTIONS ARE IGNORED.

GENERALIZED KINETICS SYNTHESIS CODE: DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY. DATE: 02/02/79

OF 36 INPUT REACTIONS SCANNED, 16 WERE RETAINED (MAXIMUM ALLOWED = 16) AND 20 WERE IGNORED FOR REASONS ITEMIZED IN THE TABLE. OF THOSE RETAINED, 8 REQUIRE RATES FROM AN E- KINETICS ANALYSIS. 18 SEPARATE SPECIES WERE ENCOUNTERED (MAXIMUM ALLOWED = 20).

ERRORS WHICH WERE DETECTED IN PROCESSING THE INPUT REACTION SCHEME MAY CAUSE PROGRAM TERMINATION IF THEY HAVE BEEN SPECIFIED TO BE TREATED AS FATAL. MODIFICATIONS OF THE REACTION SCHEME, CORRECTIONS IN REACTION SYNTAX, CHANGES IN DIMENSION STORAGE, OR ADDITIONS TO THE E- CROSS SECTION FILE MAY BE REQUIRED TO REMOVE ALL OF THE ERROR DECLARATIONS.

Fig. 4.37: Summary of defective reaction scheme (cont'd).

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
(DATE: 01/05/79)

```
CARD                1         2         3         4         5         6         7         8
 NO.     12345678901234567890123456789012345678901234567890123456789012345678901234567890
--------------------------------------------------------------------------------------------

  1 ...  $CONTROL          IO(1) = 1,1,1,1,1,1,10,0,0,1,
  2 ...                    EMAX = 20.,
  3 ...                    NCYCLE = 200,
  4 ...                    LIMIT = 5$
  5 ...  $PARAM            TPULSE = 1.0E-06,
  6 ...                    ATM = 1.7$
  7 ...  $OPTICAL          REFLECT = 70.,
  8 ...                    LOSS = 0.,
  9 ...                    AREA = 25.,
 10 ...                    CAVITY = 130.,
 11 ...                    LENGTH = 75.0$
 12 ...  $EBEAM            JBEAM = 12.0,
 13 ...                    ENERGY = 320.,
 14 ...                    UB = 20.,
 15 ...                    TB(1) = 0., 50., 100., 150., 200., 250., 300.,
 16 ...                              350., 400., 450., 500., 550., 600., 650.,
 17 ...                              700., 750., 800., 850., 900., 950., 1000.,
 18 ...                    UNITS = 1.0E-09,
 19 ...                    JB(1) = 0., .82, 1., 1., .9, .85, .77, .73, .69,
 20 ...                              .67, .69, .72, .75, .75, .72, .65, .42, .2,
 21 ...                              .05, .02, 0.,
 22 ...                    FACTOR = 2.0$
 23 ...  $CIRCUIT          CAPAC = 1.33E-06,
 24 ...                    INDUCT = 200.E-09,
 25 ...                    RESIST = 0.,
 26 ...                    KVOLT = 40.,
 27 ...                    AREA = 2000.,
 28 ...                    DIST = 10.$
 29 ...  $RATES            KF(9) = 1.,
 30 ...                    KR(12) = 1.,
 31 ...                    KF(17) = 1.E-07,
 32 ...                    KR(26) = 1.,
 33 ...                    KF(44) = 6.2E-12,6.0E-32,
 34 ...                    KR(50) = 0.$
 35 ...AR              1191.                40.
 36 ...KR               100.                84.
 37 ...F2                1.5                38.          PLOT
 38 ...AR*                        11.5
 39 ...KR*                         9.9
 40 ...AR2(*)                     13.0
--------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

CONTINUED

Fig. 4.38: DATA BLOCK 4 input for illustration of error diagnostics.

SUMMARY OF CARD IMAGES FOR INPUT DATA DECK
(DATE: 01/05/79)

```
CARD              1         2         3         4         5         6         7         8
 NO.    12345678901234567890123456789012345678901234567890123456789012345678901234567890
-------------------------------------------------------------------------------------------

 41 ....KR2(+)                    11.8
 42 ....ARKR(+)                   12.4
 43 ....AR**                      13.5
 44 ....AR(+)                     15.8
 45 ....KR**                      11.5
 46 ....KR(+)                     14.4
 47 ....F-
 48 ....ARF*                       6.5
 49 ....KRF*                       5.0
 50 ....AR2*                       9.5
 51 ....KR2*                       8.2
 52 ....AR2F*                      5.0
 53 ....ARKRF*                     4.0
 54 ....KR2F*                      3.0
 55 ....ARKR*                      8.8
 56 ....F-                        0.01
 57 ....E(-)                                          PLOT
 58 ....XXX             0.5
-------------------------------------------------------------------------------------------

        12345678901234567890123456789012345678901234567890123456789012345678901234567890
                  1         2         3         4         5         6         7         8
```

Fig. 4.38 (Continued)

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PHOCESS IN THE E- KINETICS ANALYSIS)

	I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
	1	AR + E → AR* + E	VSIG(1, 1)	VSIG(2, 1)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
	2	KR + E → KR* + E	VSIG(1, 2)	VSIG(2, 2)	SCHAPER, SCHEIBNER, BEITRAGE AUS PLASMA PHYS 9, 45
	3	AR + E → AR** + E	VSIG(1, 3)	VSIG(2, 3)	0.1 X CROSS SECTION FOR AR + E → AR* + F IS ASSUME
	4	KR + E → KR** + E	VSIG(1, 4)	VSIG(2, 4)	0.1 X CROSS SECTION FOR KR + E → KR* + F IS ASSUME
	5	AR* + E → AR** + E	VSIG(1, 5)	VSIG(2, 5)	VRIENS CROSS SECTION
	6	KR* + E → KR** + E	VSIG(1, 6)	VSIG(2, 6)	VRIENS CROSS SECTION
	7	AR + E → AR(+) + E + E	VSIG(1, 7)		D. RAPP AND P. J. ENGLANDER-GOLDEN, J CHEM PHYS 43
	8	KR + E → KR(+) + E + E	VSIG(1, 8)		KIEFFER REPORT, P. 16
**	9	AR* + E → AR(+) + E + E	VSIG(1, 9)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
	10	KR* + E → KR(+) + E + E	VSIG(1,10)		D. TON-THAT, M. R. FLANNERY, TO BE PUBLISHED
	11	AR** + E → AR(+) + E + E	VSIG(1,11)		VRIENS CROSS SECTION
**	12	KR** + E → KR(+) + E + E	VSIG(1,12)		VRIENS CROSS SECTION
	13	AR2(+) + E → AR* + AR	VSIG(1,13)		MEHR AND BIONDI: SYNTHETIC CROSS SECTION FOR TE**
	14	KR2(+) + E → KR* + KR	VSIG(1,14)		OSKAM, MITTELSTADT: SYNTHETIC, TE**(-2/3) LAW.
	15	F2 + E → F + F-	VSIG(1,15)		AEROSPACE (PRIVATE COMMUN.)
	16	AR2* + E → AR + AR + E	1.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
*	17	KR2* + E → KR + KR + E	1.0000E-07		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
	18	AR + HE- → AR(+) + HE- + E	4.3400E-18		BERGER-SELTZER: STOP = 1.7 MEVCM2/GM (300 KEV)
	19	AR + HE- → AR* + HE-	1.2400E-18	1.2400E-18	(1/3.5) X AR + HE → AR(+) + E + HE
	20	KR + HE- → KR(+) + HE- + E	8.0400E-18		BERGER-SELTZER: STOP = 1.5 MEVCM2/GM (300 KEV)

* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED
** ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme.

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

	I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
	21	KR + HE- → KR* + HE-	2.3000E-18	2.3000E-18	(1/3.5) X KR + HE → KR(+) + E + HE
	22	AR(+) + AR + M → AR2(+) + M	2.0000E-31		W. F. LIU, D. C. CONWAY JCP 62, 3070 (1975)
	23	AR(+) + KR + M → ARKR(+) + M	2.5000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
	24	KR(+) + KR + M → KR2(+) + M	2.4000E-31		C. J. TRACY, H. J. OSKAM JCP 65, 3387 (1976)
	25	KR(+) + AR + M → ARKR(+) + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
**	26	AR(+) + KR → AR + KR(+)	3.0000E-11	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	27	AR2(+) + KR → KR(+) + AR + AR	7.5000E-10		BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
	28	ARKR(+) + KR → KR2(+) + AR	3.2000E-10	X E(-E/KT)	BOHME ET AL, J. CHEM. PHYS. 52, 5094 (1970)
	29	AR* + AR + M → AR2* + M	1.0000E-32		HILL, GUTCHECK, HUESTIS, ET AL, SRI REPORT, 1974.
	30	AR* + KR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
	31	KR* + KR + M → KR2* + M	5.5000E-32		HUGHES LASL ASPEN 9/76
	32	KR* + AR + M → ARKR* + M	1.0000E-32		REVERSE REACTION IS IGNORED -- KR = 0.
	33	ARKR* + KR → KR2* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
	34	AR2(+) + F- → ARF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	35	AR2(+) + F- → AR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
	36	AR(+) + F- → ARF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
	37	KR2(+) + F- → KRF* + KR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	38	KR2(+) + F- → KR2F*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
	39	KR(+) + F- → KRF*	1.0000E-06		REVERSE REACTION IS IGNORED -- KR = 0.
	40	ARKR(+) + F- → KRF* + AR	5.0000E-07	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.

** ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme. (Continued)

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

	I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
	41	ARKR(+) + F- → ARKRF*	5.0000E-07		REVERSE REACTION IS IGNORED -- KR = 0.
	42	KR* + F2 → KRF* + F	7.2000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
	43	AR* + F2 → ARF* + F	7.5000E-10	X E(-E/KT)	VELAZCO, KOLTS, SETSER, JCP 65, 3469 (1976)
*	44	AR* + KR → AR + KR*	6.2000E-12	X E(-E/KT)	***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
*	45	KRF* + AR + M → ARKRF* + M	6.0000E-32		***** THE ORIGINAL RATE HAS BEEN MODIFIED *****
	46	KRF* + KR + M → KR2F* + M	5.0000E-31		AVCO
	47	ARF* + AR + M → AR2F* + M	4.0000E-31		AVCO
	48	ARF* + KR + M → ARKRF* + M	1.0000E-31		REVERSE REACTION IS IGNORED -- KR = 0.
	49	AR2* + KR → AR + AR + KR*	8.0000E-11		ZAMIR (PRIV. COMMUN. TO SRI)
**	50	AR2* + AR2* → AR2(+) + AR + AR + E	3.0000E-10		E- CREATED (OR LOST) ASSUMED TO BE AT ZERO ENERGY
	51	ARF* + KR → KRF* + AR	1.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
	52	AR2* + F → ARF* + AR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	53	KR2* + F → KRF* + KR	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	54	AR2* + F2 → AR2F* + F	2.5000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
	55	ARKR* + F2 → KRF* + AR + F	6.0000E-10		SRI REPORT NO. MP 76-99, DEC., 1976
	56	ARKR* + F2 → ARKRF* + F	3.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
	57	KR2* + F2 → KR2F* + F	3.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
	58	AR2F* + F2 → AR + AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
	59	ARKRF* + F2 → AR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
	60	KR2F* + F2 → KR + KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976

* THE ORIGINAL RATE CONSTANT(S) HAVE BEEN MODIFIED
** ILLEGAL ATTEMPT TO MODIFY RATE CONSTANT(S) WAS REJECTED

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme. (Continued)

SUMMARY OF UPDATED RATES FOR INPUT REACTION SCHEME OF SYNTHETIC KINETICS CODE GENERATED ON 01/04/79
DR. WILLIAM B. LACINA, NORTHROP RESEARCH AND TECHNOLOGY CENTER, PALOS VERDES, CALIFORNIA

(VSIG(K,I) ARE FORWARD (K=1) OR REVERSE (K=2) RATES FOR THE ITH INELASTIC PROCESS IN THE E- KINETICS ANALYSIS)

I	REACTION(I)	KF(I)	KR(I)	REFERENCES OR COMMENTS
61	ARKRF* + KR → KR2F* + AR	1.0000E-10	X E(-E/KT)	SRI REPORT NO. MP 76-99, DEC., 1976
62	KRF* + F2 → KR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
63	ARF* + F2 → AR + F + F2	1.0000E-09		SRI REPORT NO. MP 76-99, DEC., 1976
64	AR2F* + KR → KRF* + AR + AR	1.0000E-10		REVERSE REACTION IS IGNORED -- KR = 0.
65	AR** + M → AR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
66	KR** + M → KR* + M	1.0000E-10	X E(-E/KT)	REVERSE RATE IS OBTAINED FROM DETAILED BALANCE.
67	ARF* → AR + F	3.3000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
68	AR2* → AR + AR	3.8000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
69	ARKR* → AR + KR	3.0000E+06		REVERSE REACTION IS IGNORED -- KR = 0.
70	KR2* → KR + KR	3.3000E+06		SRI REPORT NO. MP 76-99, DEC., 1976
71	AR2F* → AR + AR + F	2.0000E+08		SRI REPORT NO. MP 76-99, DEC., 1976
72	ARKRF* → AR + KR + F	5.0000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
73	KR2F* → KR + KR + F	6.7000E+07		SRI REPORT NO. MP 76-99, DEC., 1976
74	KRF* → KR + F + HNU	1.1000E+08		R. BURNHAM, S. 5. SEARLES (SUBMITTED TO JCP)
75	KRF* + RAD → KR + F + RAD	2.0000E-16		LASER TRANSITION: STIMULATED EMISSION X-SECTION
76	F2 + RAD → F + F	1.5000E-20		REVERSE REACTION IS IGNORED -- KR = 0.
77	F- + RAD → F + E	5.4000E-18		A. MANDL, PHYS REV A3, 251 (1971)
78	KR2F* + RAD → AR* + KR + F	1.0000E-99		CROSS SECTION UNKNOWN
79	AR2(+) + RAD → AR + AR(+)	1.5000E-17		STEVENS (PARK CITY CONFERENCE)
80	KR2(+) + RAD → KR + KR(+)	3.5000E-18		J. WEST (NRTC)

Fig. 4.39: Tabular summary of modified rate constants for the kinetic reaction scheme. (Continued)

SUMMARY OF POSSIBLE ERROR CONDITIONS

SEVERITY	DESCRIPTION
WARNING:	ERRORS WERE DETECTED IN PROCESSING THE INPUT REATION SCHEME. MODIFICATIONS OF THE REACTION SCHEME, CORRECTIONS IN REACTION SYNTAX, CHANGES IN DIMENSION STORAGE, OR ADDITIONS TO THE E-CROSS SECTION FILE MAY BE REQUIRED TO REMOVE ALL OF THE ERROR CONDITIONS.
WARNING:	SYNTHESIZED SUBROUTINES AND DATA FILE WERE GENERATED WITH DIMENSION DECLARATORS NMAX = 30, KMAX = 200, AND NKMAX = 25. THESE MUST AGREE WITH THE CORRESPONDING DIMENSION DECLARATORS IN THE MAIN PROGRAM (LASER). EXECUTION MAY BE POSSIBLE IF PRESENT STORAGE EXCEEDS ORIGINAL, BUT CAUTION IS ADVIVISED TO INSURE THAT LABELED COMMON BLOCKS AGREE WITH THOSE IN THE SYNTHETIC SUBROUTINES ASSOCIATED WITH THE DATA FILE GENERATED ON TAPE4.
WARNING:	TAPE4 DATA FILE VECTORS EXCEEDED DIMENSION STORAGE IN MAIN PROGRAM, AND WERE TRUNCATED DURING READ. NKMAX = 25, KMAX = 200, AND NMAX = 30. TAPE4 CONTAINS NK = 15, KTYPE = 80, AND NTYPE = 24. CAUTION IS ADVISED.
WARNING:	AN ATTEMPT WAS MADE TO ENTER, BY $RATES ... $ INPUT, THE FOLLOWING RATES, WHICH ARE NOT ACCESSIBLE BY INPUT FOR THE SYNTHETIC PROGRAM THAT WAS GENERATED. IF THE PROGRAM EXECUTES, THE ATTEMPTED MODIFICATIONS WILL BE IGNORED, AND THE ORIGINAL RATES USED: KF(9) KR(12) KR(26) KR(50)
WARNING:	THE FOLLOWING SPECIES WERE INITIALIZED BY INPUT DATA, BUT DID NOT OCCUR IN THE KINETIC SYSTEM. IF THE PROGRAM IS EXECUTED, THEY WILL BE IGNORED, BUT INCLUDED IN THE TOTAL PRESSURE (AS BUFFER GASES IN 3-BODY COLLISIONS) AND FOR MOMENTUM TRANSFER IN E- KINETICS ANALYSIS: XXX
WARNING:	INITIAL POPULATION DENSITIES FOR THE FOLLOWING SPECIES WERE NOT DEFINED. IF THE PROGRAM IS EXECUTED, NO(I) = 0 WILL BE ASSUMED: RAD AR* KR* AR** KR** AR(+) KR(+) AR2(+) KR2(+) F F- AR2* KR2* ARKR(+) ARKR* ARF* AR2F* KRF* KR2F* ARKRF*
WARNING:	ENERGIES FOR THE FOLLOWING SPECIES WERE NOT DEFINED. IF PROGRAM IS EXECUTED, E(I) = 0 WILL BE ASSUMED: AR KR F2 F

Fig. 4.40: Execution error diagnostics illustrated.

SUMMARY OF POSSIBLE ERROR CONDITIONS

SEVERITY	DESCRIPTION
WARNING:	ERRORS OCCURRED FOR THE INPUT CROSS SECTIONS FOR THE FOLLOWING ELECTRON COLLISION PROCESSES. IF THE PROGRAM IS EXECUTED, A ZERO CROSS SECTION OVER ALL ENERGY WILL BE ASSUMED! 1) MOMENTUM TRANSFER FOR F2 NO E- CROSS SECTION DATA WAS FOUND. 2) MOMENTUM TRANSFER FOR XXX NO E- CROSS SECTION DATA WAS FOUND. THE MASS ENTERED FOR THIS SPECIES IS ≤ 0
FATAL:	MOMENTUM TRANSFER COLLISION FREQUENCY IS ZERO AT SOME POINT. E- ANALYSIS CONTAINS 1/QM TERMS.

PROGRAM IS TERMINATED FOR ERRORS SPECIFIED FATAL.

Fig. 4.40: Execution error diagnostics (continued)

5.0 REFERENCES

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