A THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THE MECHANISMS OF THE HYDROGEN-FLUORIDE PULSED CHEMICAL LASER

Dissertation for the Degree of Ph. D. MICHIGAN STATE UNIVERSITY JOSEPH J. T. HOUGH 1975



This is to certify that the

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A THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THE MECHANISMS OF THE HYDROGEN-FLUORIDE PULSED CHEMICAL LASER presented by

Joseph J. T. Hough

has been accepted towards fulfillment of the requirements for

Doctor of Philosophy degree in Mechanical Engineering

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A THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THE MECHANISMS OF THE HYDROGEN-FLUORIDE PULSED CHEMICAL LASER

by

Joseph J. T. Hough

Kinetic mechanisms in the pulsed HF chemical laser are examined by comparing predictions from improved theoretical models with experimental observations. Additional insight into these mechanisms is obtained by examining the predictions of the models in regions outside the domain of the present experiments.

Two rate-equation models are developed for the $F + H_2$ and $F_2 + H_2$ lasers. Both models simulate cavity transients such as the interaction of the chemical kinetic and radiative phenomena within the active medium in the pulsed HF chemical laser. Calculations show that the growth in intensity is sufficiently slow that the gain may attain levels far above threshold before lasing begins. Intensity increases sharply after the gain is far above threshold, which causes the gain to drop rapidly and oscillate near the threshold value. This fluctuation in gain, which is a result of fluctuation in HF(v, J) populations, makes the calculations more sensitive to relaxation processes than has been shown by earlier constant-gain models. The model of the $F + H_2$ laser is further expanded to study the effects of preferential pumping into rotational levels, rotational relaxation, and rotational nonequilibrium. Rotational relaxation is modeled by associating with each (v, J) state a relaxation time constant (τ) consistent with available experimental data and theoretical calculations. The results show that, as the rotational relaxation rate decreases, the laser output decreases and pulse energy is more uniformly distributed among the lasing transitions within a given band. The predicted time-resolved spectrum exhibits strong simultaneous lasing on many vibrationalrotational transitions. The model is capable of predicting the performance of lasers operating in the line-selected mode. A comparison is made of the output from a three-transition cascade with the same three transitions operated in the single-line mode. The sum of the output from the three single-line calculations is 65% of the output from the cascade.

Concurrent with the theoretical work, output from an electrically initiated, transverse pin discharge SF_6-H_2 pulsed laser was characterized with model predictions, and the results are in good agreement. Experiments were conducted to investigate the effect of cavity losses and cavity threshold on the performance of the laser operating in the single line as well as the multiline mode. Losses within the optical cavity as small as 5%, typical of many lasers, can easily result in a 30% reduction of output power. This is especially significant for high-Q cavities. Model predictions graphically illustrate the effect of cavity threshold on laser output. These results should be helpful in the design of line-selected extraction techniques for high-power, pulsed (and continuous) HF lasers.

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1. INTRODUCTION

1.1 History

The basic principles of laser (or optical maser) action have been well understood since the early days of quantum theory and were clearly enunciated by Einstein in his paper on the quantum theory of radiation.¹ It was not until much later, however, that its practical significance became clear. The first successful maser was developed by Townes² at Columbia University in 1954. It was a gaseous ammonia maser that operated in the microwave range. In 1958, Schawlow and Townes³ proposed an extension of the microwave technique to the infrared and optical range, and the laser was born.

In 1960, Maiman^{4,5} published experimental results for the first succesful laser, a ruby laser. By 1972, laser action had been achieved with atoms, ions, and molecules in gases, liquids, solids, glasses, flames, plastics, and semiconductors.⁶

The characteristics of the laser, with its unique capability of delivering intense, coherent electromagnetic radiation, make it a valuable tool in the laboratory. Its temporal and spatial coherence properties have been exploited in such applications as inteferometry and holography, and made it possible to focus the laser output into an extremely small spot size, attaining power densities not possible with any other source of light. The laser quickly became a valuable tool in industry as well. In 1965, Western

Electric announced the first use of laser light in a mass production application: They had developed a laser system that could pierce holes in diamond dies for drawing wire. Industry is now using the laser to measure process parameters, scribe, drill, evaporate, and weld, in a variety of applications.⁷

Recognition of the advantages and potential of the conversion of chemical energy to laser power has brought about increased interest in the development of chemical lasers. The chemical laser is unique because it is capable of yielding very-high specific power densities with reaction initiation energies much less than those emitted in the laser beam. In other laser systems, the population inversion necessary for laser action must be achieved through the initiation energy, but in the chemical laser, the initiation energy only serves to prepare chemical species that react exothermically to produce the laser active medium. Solid-state lasers have achieved output energies of ≦5% of the initiation energy, while the CO₂ gas laser has demonstrated an initiation efficiency of as high as 25%. Chemical lasers, on the other hand, have been operated with ≥170% initiation efficiency. ⁸, ⁹

The first chemical laser was demonstrated in 1965 by Kasper and Pimentel.¹⁰ it was a flashlamp-initiated, pulsed HCl laser pumped by the reaction

$$H + Cl_2 \rightarrow HCl(v) + Cl \qquad (\Delta H = -45.2 \text{ kcal/mol}) \qquad (1.1)$$

where ΔH is the net change in molar enthalpy of the chemical system resulting from this reaction. Thereafter, a great many other

compounds were made to lase, although most of the effort has been directed toward diatomics of the hydrogen halide type. These molecules are favored because they are generally produced by highly exothermic reactions and are, thus, capable of achieving the population inversion of the vibrational levels necessary for lasing to occur. Furthermore, they have large electric dipole moments, which results in large cross sections for stimulated emission. ^{11, 12}

Laser action from the HF molecule initiated by flash photolysis of UF₆-H₂ mixtures was reported by Kompa and Pimentel¹³ shortly after the initial operation of the HCl chemical laser. At about the same time, Deutsch¹⁴ reported similar laser action resulting from the initiation by pulsed electrical discharge of SF_6 -H₂ mixtures. Both lasers were pumped by the reaction

 $F + H_2 \rightarrow HF(v) + H$ ($\Delta H = -31.7 \text{ kcal/mol}$) (1.2)

which produced a population inversion ratio¹⁵ of $N_1:N_2:N_3 = 0.31$: 1.00:0.47, where N_v represents the population of HF molecules in the vibrational level (v).

With the discovery of the chemical laser, it was recognized that one essential advantage of this laser was its potential for high efficiency, and that this efficiency could be realized through the use of a chain reaction to achieve the population inversion. The first chemical laser operating on a chain reaction was, again, the HCl laser. In 1969, Batovskii¹⁶ and Basov¹⁷ separately reported the first HF chain-reaction lasers, which were initiated by electrical discharge and flash photolysis, respectively, in mixtures of H₂

and F $_2$ gases. The chain consists of a cold reaction, Reaction (1.2), and a hot reaction,

$$H + F_2 \rightarrow HF(v) + H$$
 ($\Delta H = -97.9 \text{ kcal/mol}$) (1.3)

where the adjectives cold and hot refer to the relative exothermicity of the reactions. The population inversion ratio of Reaction (1.3)has been measured by Jonathan¹⁸ and Polanyi¹⁹ and has a maximum at v = 6.

Many other researchers subsequently investigated the H2 + F2 chain-reaction laser. Both theoretical and experimental studies were carried out. Many initiation techniques, e.g., electron-beamirradiated discharge, electrical discharge, flash photolysis, and laser photolysis, with a large assortment of experimental apparatus and a variety of gas mixing procedures were employed to obtain a wide range of results. The highest energy output (2360 J) and initiation efficiency (> 170%) attained to date were reported by Greiner et al. , 9 who utilized relativistic electron beams for initiation. Kerber et al.⁸ also obtained 170% initiation efficiency with a laser initiated by electrical discharge. Current efforts in high-energy pulsed systems are directed toward achieving successful large-volume initiation of the laser medium. The electron beam is considered a prime candidate for accomplishing this objective because of its ability to deposit large amounts of energy uniformly over a large volume of the gas mixture. 20

Although both the HF and HCl laser systems have been the subject of much research activity, the $H_2 + F_2$ laser is generally

preferred to the $H_2 + Cl_2$ laser because of the significantly higher exothermicity of the $H_2 + F_2$ chain (one reaction of the $H_2 + Cl_2$ chain is actually slightly endothermic). In addition, the HF deuterated analogue, DF, has its transitions in a transmission window of the atmosphere. Knowledge gained from the study of the HF system will facilitate the understanding of the DF system at a fraction of the cost that would otherwise be incurred in direct investigations of that system.

1.2 Present Work

Current efforts to improve the performance of the HF laser requires an understanding of the detailed mechanisms within this device. It is the purpose of this thesis to make a systematic and detailed investigation of the competing mechanisms in the pulsed HF chemical laser utilizing both the theoretical predictions of a rateequation model and laboratory observations. The specific objective of this study is to examine the kinetic mechanisms and the effect of the following:

- 1. The transient behavior of the laser parameters, which includes the interaction of gain and intensity before and during lasing.
- Nonlinear deactivation mechanisms, specifically, the vibration-vibration (VV) energy transfer process.
- 3. Laser performance as a function of level of initiation.
 - 4. Rotational nonequilibrium resulting from lasing and preferential pumping into rotational levels.
 - 5. The effect of cavity losses and cavity threshold on the output of the SF₆-H₂ laser.

Several theoretical models for the analysis of the H_2 + $F_2^{11,21-26}$ and the SF_6 - H_2^{27} chemical lasers have already been developed. These models follow the assumption that lasing begins

when gain reaches threshold and that gain equals loss during the lasing period. It has been shown, however, that rate-equation solutions of laser performance with the constant-gain assumption will minimize the effect of the very fast VV exchange reactions.^{23,25} The model presented here is similar to that of Rockwood et al.,²⁸ which was developed for pulsed CO laser simulation. Model features include the determination of the time evolution of the gain, intensities, and species concentrations. This formulation permits the observation of the time history of the interaction of gain and intensity. Since the gain levels are permitted to fluctuate in a more realistic manner than in constant-gain solutions, the modeling of nonlinear deactivation mechanisms is more accurate. This model, therefore, permits a more careful evaluation of the effect of the VV energy transfer process.

The time-resolved spectral output of the experimental data from Suchard et al.²⁹ is compared with the calculations of the computer model from Kerber et al.²³ in Figure 1.1. The V and J on the ordinate designate the lower level quantum numbers of the transitions, and the horizontal bars represent the periods of lasing on these transitions. The calculations predict a rigid J-shifting pattern and no multiline lasing, whereas the experimental data indicate significant deviation from the J shifting and definite multiline lasing.^{*} Multiline lasing was also seen in the work reported in References 30-32. The model of Reference 23 assumes a Boltzmann distribution of the rotational states at the translational temperature; the effects of preferential

The discrepancy in pulse duration has been removed by a later study, 26 in which revised kinetic rate coefficients were used.



Figure 1.1.

Comparison of time-resolved spectral output. (a) Experimental data reported in Reference 29 for a 1 $H_{2:1}$ $F_{2:60}$ He mixture at 50 Torr; (b) calculated spectrum for the same mixture from Reference 23 where rotational equilibrium was assumed. pumping and rotational hole-burning resulting from lasing are ignored. This is also true of the other existing models. The conjecture here is that rotational nonequilibrium does, in fact, exist and is the result of lasing and preferential pumping. By taking into account the effects of these two mechanisms, the present model will attempt to resolve these discrepancies.

In the following sections, the model is presented in its sequential phases of development. In the initial phase, an $H_2 + F_2$ model is formulated in which a Boltzmann distribution for the rotational states is assumed. It is compared with earlier model calculations of Kerber et al.²³ in order to illustrate the effects of the present model assumptions. Other model features are also discussed, including the cavity transients and predictions of laser performance as a function of level of initiation, using the recent chemical kinetic rate coefficients suggested by Cohen.³³

In the subsequent phases of development, the model includes the effects of rotational nonequilibrium. Unfortunately, this endeavor also increases the complexity of the model considerably, and makes the numerical computations longer than is desirable. The model is, therefore, limited to the simpler case of the SF_6-H_2 laser. For this model, the individual rotational level populations are determined from the solution of rate equations. Relaxation of the rotational population is accomplished by the assumption of a characteristic rotationalrelaxation time similar to the model of $Schappert^{34}$ for CO_2 . With the rotational populations of the first four vibrational levels identified, an accurate assessment of the effect of rotational nonequilibrium on laser performance can be made. Calculations were made to assess the effect of several rotational-relaxation rates on the spectral output of the laser.

The effect of preferential pumping into rotational levels is also considered. This formulation permits, for the first time, the study of a laser operating in the line-selected mode; the effect of cascading is evident from the results of these calculations.

An SF₆-H₂ laser was constructed in order to make an experimental check of the model predictions. Reaction of the SF₆-H₂-He (diluent) gas mixture is initiated by a helical array of electrical discharges; pulsed high voltage is supplied through the use of a triggered spark gap and a capacitor. The results are presented of an experimental and theoretical investigation conducted to assess the effect of cavity losses and cavity threshold on the performance of this device. Model predictions of laser performance are compared with experimental data, and the validity of the model assumptions is examined.

2. COMPUTER SIMULATION OF PULSED HF CHEMICAL LASER

2.1 Model Formulation

The formulation of the chemical laser computer simulation is described. A general model was developed and then tailored to the two particular cases of concern. The reactions used to represent the chemical processes are:

1. The $H_2 + F_2$ chain the within a lord are assumed to have low initial states above directed to the same rates above directed to the same rate above directed to the same rates above directed to

 $F + H_2 \rightleftharpoons HF(v) + H$

 $H + F_2 \rightleftharpoons HF(v) + F$

2. Vibrational-translational (VT) deactivation

 $HF(v) + M \rightleftharpoons HF(v') + M$

$$H_2(v) + M \rightleftharpoons H_2(v - 1) + M$$

3. VV quantum exchange

 $HF(v) + HF(v') \rightleftharpoons HF(v + 1) + HF(v' - 1)$

$$HF(v) + H_2(v') \rightleftharpoons HF(v + 1) + H_2(v' - 1)$$

4. Dissociation-recombination

 $F_2 + M \rightleftharpoons M + F + F$ $H_2 + M \rightleftharpoons M + H + H$

$$HF + M \rightleftharpoons M + H + F$$

The major provisions in the models are:

- 1. The dominant kinetic processes are represented by the reaction system suggested by Cohen³³ (Table A. 1).
- 2. The reacting mixture is homogeneous and is contained in a Fabry-Perot laser cavity.
- 3. All possible transitions within a band are assumed to have low initial intensities that grow if the gain rises above threshold. Lasing is always assumed to be in the P branch. Initial intensity levels can be selected individually or set proportional to the spontaneous emission rate.
- 4. Initiation is modeled by the introduction of a finite concentration of F atoms into the gas mixture.

The chemical reactions are written

$$\sum_{i} \alpha_{ri} N_{i} \frac{k_{r}}{k_{-r}} \sum_{i} \beta_{ri} N_{i}$$
(2.1)

where N_i is the molar concentration of species i, α_{ri} and β_{ri} are stoichiometric coefficients, and k_r and k_{-r} are forward and backward rate coefficients. The rate of change of concentration for nonlasing molecules is

$$\frac{dN_i}{dt} = X_i$$
 (2.2.a)

and, for HF molecules, one has

$$\frac{dN_{HF}(v, J)}{dt} = X_{i} + X_{rad}(v, J) - X_{rad}(v - 1, J_{L}) + A(v, J)$$
(2.2.b)

where the X_{rad} terms are rates of change in concentration as a result of lasing into and out of level (v, J). The lower-level rotational quantum numbers are J and J_L for the transitions $v + 1 \rightarrow v$ and $v \rightarrow v - 1$, respectively. The net rate of spontaneous emission into level (v, J) is given by A(v, J). The chemical reactions yield a concentration change

$$X_{i} = \sum_{r} (\beta_{ri} - \alpha_{ri}) \left(k_{r} \prod_{j} N_{j}^{\alpha_{rj}} - k_{-r} \prod_{j} N_{j}^{\beta_{rj}} \right)$$
(2.3)

and

$$X_{rad}(v, J) = g(v, J) f(v, J)$$
 (2.4)

where g(v, J) is the gain on the $v + 1 \rightarrow v$ transition with lower-level J and f(v, J) is the lasing flux on the same transition. The rate equation for the lasing flux is (Appendix B)

$$\frac{df(v, J)}{dt} = c[g(v, J) - \alpha_{thr}] f(v, J)$$
(2.5)

where c is the speed of light and

$$\alpha_{\text{thr}} = -\frac{1}{2L} \ln(R_0 R_L)$$
 (2.6)

where L is the length of the active medium and R_0 and R_L are the mirror reflectivities. The gain is²³

$$g(\mathbf{v}, \mathbf{J}) = \frac{hN_{A}}{4\pi} \omega_{c}(\mathbf{v}, \mathbf{J}) \phi(\mathbf{v}, \mathbf{J}) B(\mathbf{v}, \mathbf{J})$$

$$\times \left[\left(\frac{2J+1}{2J-1} \right) N_{HF}(\mathbf{v}+1, J-1) - N_{HF}(\mathbf{v}, J) \right] \qquad (2.7)$$

where $\omega_{c}(v, J)$ is the wave number of the transition, B(v, J) is the Einstein isotropic absorption coefficient based on the intensity, and $\phi(v, J)$ is the Voigt profile at line center as given in Reference 22. The first term of Equation (2.5) determines the rate of increase in the intensity of the radiation field within the laser cavity; the second term gives the rate energy is lost from the cavity. The lost energy includes that extracted through the output coupler as laser output as well as real losses resulting from such mechanisms as absorption, scattering, and extraneous reflections.

The energy equation for a constant density gas is

$$\sum_{i} N_{i} C_{v_{i}} \frac{dT}{dt} = -P_{L} - \sum_{i} \frac{dN_{i}}{dt} H_{i}$$
(2.8)

where $C_{v_{\underline{i}}}$ is the molar specific heat at constant volume, $H_{\underline{i}}$ is the molar enthalpy of species i, and $P_{\underline{L}}$ is the output lasing power per unit volume. The output power in the $v + 1 \rightarrow v$ band is

$$P_{Lv}(t) = \sum_{j} hc N_A \alpha_{thr} \omega_c(v, J) f(v, J)$$
(2.9.a)

$$P_{L}(t) = \sum_{v} P_{Lv}(t)$$
 (2.9.b)

where the only cavity loss is assumed to be the laser output. In making comparisons with experimental measurements, however, real losses must be accounted for, as discussed in Chapter 3 and Appendix E.

Numerical integration of Equations (2. 2), (2. 5), and (2. 8) by the modified Adams-Moulten method of Gear³⁵ determines the time evolution of the species concentrations, temperature, pressure, the gain on all transitions, and the intensities on all lasing transitions. The laser energy extracted in each band is then determined by integrating the power

$$\mathbf{E}_{\mathbf{v}} = \int_{0}^{\mathbf{t}_{\mathbf{c}}} \mathbf{P}_{\mathbf{L}\mathbf{v}} \, \mathrm{dt}$$
 (2.10.a)

where t is the length of laser pulse and the total pulse energy is

$$E = \sum_{v} E_{v}$$
 (2.10.b)

2.2 Effect of Relaxation Oscillations

The term "relaxation oscillation" frequently has been used to describe the phenomenon that results from gain fluctuations during pulsed-laser operation. In this section, the results of computations of the performance of a laser pumped by the $H_2 + F_2$ chain reaction are given. These results are compared with those of the model of Reference 23, and the unique features of the present model are

and phically illustrated. In this for colstion, a Holtanana distribution

graphically illustrated. In this formulation, a Boltzmann distribution for the rotational populations at the translational temperature is assumed; hence,

$$N_{HF}(v, J) = N_{HF}(v) \left[\frac{2J+i}{Q_r^v(T)} \right] e^{-hcE_J^v/kT}$$
(2.11)

where the values of the rotational partition function $Q_{\mathbf{r}}^{\mathbf{r}}(\mathbf{T})$ and the rotational energy $\mathbf{E}_{\mathbf{J}}^{\mathbf{r}}$ are from the data of Mann et al. ³⁶

2.2.1 Comparison with Existing Models

The most extensive calculations of pulsed $H_2 + F_2$ chainreaction chemical laser performance have been made by Kerber et al. ²³ by means of the constant-gain model. ²² The present model predictions are compared with those of Reference 23. Comparisons are made by the use of the same chemical equations and rate coefficients given in Table II of Reference 23.

In Figure 2.1, a comparison is shown of power histories as computed from both models for the case F:F₂:H₂:A_r = 0.1:1:1:50 at an initial pressure (P₁) of 1.207 atm and an initial temperature (T₁) of 300°K. The cavity conditions were set at R₀ = 0.8, R_L = 1.0, and L = 100 cm. In general, the predicted pulse shape and pulse duration of the two models are comparable. The small fluctuations resulting from J-shifting in the model of Reference 23 were deleted in their figure. However, it is clear that the characteristics of the present model facilitate simulation of power fluctuations and that these fluctuations are significant during at least half of the pulse. This is even more graphically illustrated when the results of



Figure 2.1. Comparison of power histories as determined by present model and by constant-gain model, 23

Reference 23 for the power on the 2-1 band are compared with those of the present model in Figure 2.2.a. In this figure, the details of the fluctuations from the constant-gain solution are plotted without smoothing. In Figure 2.2.b, the time evolution of the laser intensity on the various transitions in the P_{2-1} band is shown. The present model permits simultaneous lasing on all transitions that reach threshold; however, the present assumption of rotational equilibrium causes J-shifting in the manner shown in the earlier models. Previous models show lasing only on the transition with maximum gain. Lasing output spectra are found to be on lower J levels than the J levels of Reference 23; this result is more consistent with experiment. ³⁰ Actual laser performance often exhibits the more erratic oscillations predicted by the present model; this is confirmed by the pulse profiles given in References 8 and 26.

The small-signal gain of the standard case from Reference 23 was compared with that calculated by use of the present model to check the thermodynamic, spectroscopic, and kinetic data. These results compare to within 1%. The effect of including spontaneous emission on the small-signal gain is less than 3%.

Since the rate of relaxation of HF(v) by VV processes is proportional to [HF(v)][HF(v')], these rates are nonlinear with respect to excited HF populations. With this in mind, the time evolution of the gain of selected transitions of the present model is compared in Figure 2.3 with that of the constant-gain model of Reference 23. The significance of the constant-gain assumption is the prediction of lower inversions, and thereby the effect of deactivation mechanisms is minimized.



Figure 2.2. Model calculations of power histories of 2-1 band. (a) comparison of the predictions of the present model with that of the constant-gain model; (b) individual transitions in the 2-1 band as determined from the present model.



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Comparation of third this rejot gain for arbitrate 3 , transitions of standard cases as modeled in present model and in constant/gain model of Keteranes 23, for the $2^{\rm (0)}$ (6) $P_2((0), (c), P_2((1)), (c), P_2((1)), Exact time hits where for the constant of the time standard the the time standard the time sta$

Figure 3. 1

Figure 2.3. Comparison of time history of gain for selected transitions of standard case as modeled in present model and in constant-gain model of Reference 23.
(a) P₂(9), (b) P₂(10), (c) P₂(11). Exact time histories for the constant-gain model for the times when the gain is less than threshold were not available; therefore, these portions of the curves are shown schematically.

10-2 PRESENT MODEL THRESHOLD the intensity drops 10⁻³ CONSTANT-GAIN MODEL 10-4 1 2 3 (a) Constant-pain model 10⁻² PRESENT MODEL ່ຮູ THRESHOLD 10-3 GAIN, CONSTANT-GAIN MODEL sensitivity, is is an 10 1 2 3 (b) for an around ran 10-2 PRESENT MODEL THRESHOLD 10-3 CONSTANT-MODEL 10-4 0 1 2 3 (c) higher than assumed in the art TIME, #sec

Figure 2.3

The onlys calculate

The results from the two models for the standard case and for the same case with the HF-HF VV rates increased by one hundred are compared in Table 2.1. The pulse duration (t,) is the time at which the intensity drops to 1% of its peak value, and $t_{1/2}$ is the time required to release one-half of the total pulse energy. Since the present model predicts gain to be significantly above threshold, HF(v) concentrations attain values well above those predicted by the constant-gain model. Therefore, the role of HF vibrational relaxation and the associated losses show a more pronounced effect in the present model. This is evident in Table 2.1 for selected VV rates. Although energy is extracted from the laser at approximately the same rate in both models (compare $t_{1/2}$), the present model shows a much earlier pulse termination. Since the model exhibits this sensitivity, it is appropriate to examine the effect of VV relaxation for an assumed rate equal to the bimolecular gas collision rate (collision diameter (d) = 3 Å). The model predictions with this rate are also shown in Table 2.1. A much higher portion of the pulse energy is found in the upper bands for this case. Further investigation indicated that this distribution of energy among the various bands varies with cavity loss (α_{thr}) . It is important to note that recent experiments by Bott³⁷ indicate that the VV relaxation rate is much higher than assumed in the standard rate of Reference 23. This new rate is incorporated into the kinetic model of Cohen³³ in Table A. 1 of Appendix A.

The pulse calculated for the second case studied in depth in Reference 23, with an initial mixture $F:F_{2}:H_{2}:Ar = 0.01:1:1:50$ at 1.207 atm and 300°K and the cavity conditions the same as previously
Effect of HF VV rate coefficient change on model predictions Table 2.1.

| ime, µsec | 1 t _{1/2} | tie i tous | 1 1.0 | 0 1.0 | - | 2 1.0 | 0 1.0 | 2 1.1 |
|---------------------------|--------------------|-------------------------------------|----------|------------|-----------------------------------|----------|------------|-------------------|
| Ti | E | 24, 21 () | 0.101 4. | 0.107 4. | | 0.089 3. | 0.096 3. | 0.110 3. |
| ine | E65 | bions. | 0.0048 | 0.0049 | | 0.0041 | 0.0041 | 0.0054 |
| cc | E54 | lel | 0.0109 | 0.0112 | 2.0 | 0.0095 | 0.0095 | 0.0136 |
| lergy, J/ | E43 | -Gain Moo | 0.0115 | 0.0123 | nt Model | 0.0092 | 0.0102 | 0.0266 |
| Er | E32 | Constant- | 0.0195 | 0.0235 | Prese | 0.0164 | 0.0212 | 0.0334 |
| Ti a | E21 | n ar | 0.0337 | 0.0400 | 14 | 0.0310 | 0.0373 | 0.0272 |
| ow, | E10 | v at | 0.0208 | 0.0151 | ri, | 0.0184 | 0.0131 | 0.0044 |
| the the Ti togic | Rate | a th twh type tog 9) 11 | Standard | High VV HF | y du g es own dip uis | Standard | High VV HF | Gas Kinetic VV HF |

used, indicates the presence of relaxation oscillations similar to that shown in Figure 2.1. However, as the characteristic times of the chemical kinetic and radiation processes decrease relative to the period of one round trip in the cavity, the effect of these oscillations decreases. Therefore, as the level of initiation in the chemical laser decreases, which implies F/F_2 initial decreases, the effect of the additional features of the present model diminish. Even in this range, the additional information contained in the prediction of the time evolution of the gain and intensity on each transition makes these calculations instructive.

2.2.2 Other Model Features

For all the calculations presented, the initial photon flux was set at 10^{-14} mol/cm². For reductions in this flux of as much as 10^{-3} , the pulse length changed by less than 1% and the pulse energy changed by less than 3%. Therefore, the calculations are relatively insensitive to the initial flux levels. If desired, these flux values may be set proportional to the rate of spontaneous emission.

The gain and intensity profile of the $P_2(10)$ line are shown in Figure 2.4. When the gain reaches threshold, the intensity begins to grow, slowly at first; but, since its growth is nonlinear, the rise becomes sharp as gain and intensity become larger. The resulting high flux causes the gain to drop below threshold and to oscillate near that value while lasing continues.

The gain profile shows several other "dips" before the $P_2(10)$ line begins lasing. These dips are caused by lasing on the $P_2(7)$, $P_2(8)$, and $P_2(9)$ lines. This is to be expected since the depopulation of a J-level as a result of lasing must be "shared" by other rotational



Figure 2.4. Time evolution of gain and output power for $P_2(10)$ transition for standard case.

levels to maintain the Boltzmann distribution. This loss of population in the upper level causes a drop in the gain profile of all the J-levels. Those nearest the lasing J are most significantly affected, even though the Boltzmann distribution is maintained. This is also the reason for the termination of the $P_2(10)$ line. As the $P_2(11)$ line begins to lase, there is a drop in the gain profile of all J-levels. The $P_2(10)$ line is already at threshold gain, and the drop causes gain to fall far below threshold and lasing terminates. Hence, if a Boltzmann distribution for the rotational levels is assumed, there is not an extensive amount of simultaneous lasing among the J-levels of a given band. The intensity profiles of the $P_2(J)$ lines are shown in Figure 2.2.b. Although the gain reaches values well above threshold, a total population inversion has never been observed; therefore, lasing on the R-branch is not possible.

The kinetic model recently reviewed by Cohen³³ has been used to study the effect of the initial F/F_2 ratio on pulse energy and pulse duration as shown in Figures 2.5 and 2.6, respectively. The initial F-atom concentration is varied while the stoichiometric balance is maintained between H and F. Other initial conditions are held constant. The initial gas mixture is $YF:1H_2:XF_2:50He$ with 2X + Y = 2. The initial temperature and pressure are 300° K and 50 Torr, respectively. The cavity parameters are set at $R_0 = 0.8$, $R_L = 1.0$, and L = 100 cm. For the specific mixture and cavity conditions considered, the present calculations indicate that the maximum pulse energy will be obtained at initial F/F_2 concentrations of approximately 0.15. For the more preliminary kinetic model of Reference 23, this optimum occurred at a ratio of F/F_2 of approximately 0.4.



Figure 2.5. Effect of initial F₂ dissociation on pulse energy and initiation efficiency as computed with recent rate coefficient compilation of Cohen. ²⁹



Figure 2.6. Effect of initial F₂ dissociation on pulse length as computed with recent rate coefficient compilation of Cohen²

In Figure 2.5, the ratio of pulse energy to the energy required to produce the initial F-atom concentration by dissociation of F_2 is also shown. Model calculations become very long and expensive as the ratio F/F_2 is decreased; therefore, an optimum point was not determined. Note, however, that this ratio is still increasing sharply with decreasing F/F_2 at a ratio equal to 0.016. The particular optimum for this curve is, of course, very dependent upon mixture composition and cavity parameters.

The variation of the pulse time parameters shown in Figure 2.6 is similar to that presented in Reference 23.

2.3 Effect of Rotational Nonequilibrium

The significance of rotational relaxation on the characteristics of laser performance was investigated. Because of the complexity of the calculations, the study was restricted to the simpler case of the SF_6 - H_2 laser. Since the model was developed to compare with subsequent experiments, some features of the model are peculiar to that purpose.

The laser cavity is assumed initially to contain a homogeneous mixture of H_2 and SF_6 . Since less than 5% of the SF_6 is typically consumed during the discharge, ³⁸ it is treated strictly as a diluent, and the net result of the F-atom producing plasma kinetics is incorporated separately. ^{*} Lyman²⁷ found the F-atom production rate to

[&]quot;This model, therefore, does not incorporate deactivation by ions, at least one of which, F", is considered significant. (J. S. Whittier, The Aerospace Corporation, private communication, March 1974).

be roughly proportional to the input power. This proportionality is assumed in this study. The contribution of the input power to the translational temperature rise is also included. The kinetic processes are the same as in the preceding $H_2 + F_2$ model, except that only the $F + H_2$ reaction is considered and the diluents are different. Since the model formulation is the same as that previously used, with the exception of the initiation simulation and the rotational relaxation feature, the details will not be repeated.

Rotational relaxation is incorporated into the model by associating a relaxation time constant, $\tau(v, J)$, with each HF(v, J) state. These constants are formulated such that their characteristics are consistent with available experimental and theoretical data concerning the relaxation mechanism. This formulation permits a straightforward analysis of the dependence of rotational relaxation without resorting to the detailed molecular collision dynamics, and it provides a simple approach to evaluating the broad effects of rotational nonequilibrium in the lasing process.

Available experimental data on rotational-relaxation time constants are generally the result of analysis of acoustic absorption or thermal conductivity measurements. * A partial compilation of

Several laboratories are presently conducting experiments to measure HF rotational-relaxation rates. Techniques such as chemiluminescence (T. L. Cool, Cornell University, Ithaca, New York), single-pulse pump-probe with a Pocket's cell used for optical switching ³⁹ and double resonance 40 are used. Because of frequency coincidence problems, the double resonance results are of dubious value. No results are yet available from the chemiluminescence studies. The pump-probe technique gave k_{HF-HF} = (7.8 ± 0.2) × 10⁷ sec⁻¹ Torr⁻¹ and (4.9 ± 0.4) × 10⁷ sec⁻¹ Torr⁻¹ for the self-relaxation rates of the P₄(5) and P₁(6) transitions, respectively.

existing data are given in References 41 and 42. Although all measurements are not in agreement, most concur with the following observations:

- 1. The rotational relaxation time constant (τ_R) increases for decreasing moment of inertia. 41, 42
- 2. TR increases for decreasing dipole moment. 41,42
- 3. TR increases for increasing temperature. 43-47

Tp is defined by

$$\frac{\mathrm{d}\mathbf{E}_{\mathrm{R}}}{\mathrm{d}\mathbf{t}} = \frac{\mathbf{E}_{\mathrm{R}}(\mathrm{T}) - \mathbf{E}_{\mathrm{R}}(\mathrm{t})}{\tau_{\mathrm{R}}}$$
(2.12)

where $E_R(T)$ is the rotational energy of the system in equilibrium at temperature (T) and $E_R(t)$ is that energy at time (t). Strictly speaking, this equation is valid only for small departures from equilibrium. Raff and Winter, ⁴⁵ and more recently Polanyi and Woodall, ⁴⁸ have developed rate-equation models that describe rotational relaxation in which rate coefficients depend upon the rotational energy separation. Their results indicate that it is insufficient to associate a relaxation time with each vibrational level; instead, one such parameter, $\tau(v, J)$, is necessary for each vibrational-rotational state.

If $\tau(\mathbf{v}, \mathbf{J})$ were assumed to be an increasing function of the rotational energy separation $(\Delta \mathbf{E}_{\mathbf{v}, \mathbf{J}})$, the first and third observations would be satisfied. Such an assumption is realistic since, for the increasing energy separation between adjacent levels, the probability of a collision being energetic enough for energy transfer to occur is decreased. A discussion of the consistency with these observations follows.

For a rigid rotor,

$$\Delta E_{I} = E_{I+1} - E_{I}$$
 (2.13.a)

and

$$\Delta E_{J} = h^{2} \frac{(J+1)}{4\pi^{2}I}$$
 (2.13.b)

which shows that ΔE_{T} increases linearly with the rotational quantum number J and is inversely proportional to the moment of inertia of the molecule. Hence, as I is decreased, ΔE_{τ} and $\tau(v, J)$ increase. Similarly, as temperature is increased, the higher J-states become more populated, and the larger $\tau(v, J)$ associated with these higher J-states become important in the overall equilibrium process. Thus, the time scale for relaxation increases. Although this argument is specifically for a rigid rotor, it is clear that a similar argument may be used for the general case. When it is considered that a smaller dipole moment implies a decrease in the interaction cross section, it is not surprising that τ_p increases for a decreasing dipole moment. Polanyi and Woodall⁴⁸ ignored this in their computations of rotational relaxation of HCl. and still obtained excellent results. This effect is also neglected in this study. Under extreme conditions of rotational nonequilibrium, J-J lasing may contribute to the relaxation process. This effect has also been neglected.

There are two processes that contribute to the perturbation of the equilibrium among the rotational states: lasing and preferential pumping. It is assumed that the vibrational-relaxation process will not disturb the rotational equilibrium since it is a relatively slow process. The rate equation for the HF(v, J) populations, i.e., Equation (2.2.b), is modified to

$$\frac{dN_{HF}(v, J)}{dt} = P(v, J) + B(v, J) R(v) + g(v, J) f(v, J)$$

$$- g(v - 1, J + 1) f(v - 1, J + 1) + \frac{N_{HF}^{B}(v, J) - N_{HF}(v, J)}{\tau_{R}(v, J)}$$
(2.14)

where P(v, J) is the pumping rate into level (v, J), R(v) is the net rate of vibrational relaxation into level v, B(v, J) is the Boltzmann rotational distribution at (v, J) for unit concentration, $N_{NF(v, J)}^{B}$ is the instantaneous rotationally equilibrated concentration of the level (v, J), and $\tau_{R}(v, J)$ is the time constant of rotational relaxation for level (v, J). Although some experimental data concerning P(v, J) are available, ^{15, 49} they are far from complete. Monte Carlo trajectory calculations have been made by Muckerman, ⁵⁰ Blais and Truhlar, ⁵¹ and Wilkins. ⁵² For this study, the computations of Wilkins are used; a linear fit of his results at 300 and 500°K is assumed, and a check is made of the effect of this assumption. The relaxation time, $\tau_{R}(v, J)$, is assumed to be of the form

$$\tau_{R}(v, J) = A_{\tau} e^{B\Delta E} v, J^{/kT}$$
(2.15)

where A_{τ}^{-1} is selected as some fraction of the binary collision frequency and B is a parametric constant in the exponential that further approximates the transition probability of the collisions. For this study, B is set at 1.0 × 10⁻³. The initiation energy is added to the energy equation to yield

$$\sum_{i} N_{i} C_{v_{i}} \frac{dT}{dt} = P_{I} - P_{L} - \sum_{i} \frac{dN_{i}}{dt} H_{i}$$
(2.16)

where P_I is the input power. This model evaluates the time history of concentration corresponding to the first sixteen rotational states of the lower four vibrational states. The resulting set of nonlinear first-order ordinary differential equations are solved by the same modified Adams-Moulten technique used earlier.

Model calculations were made at various rotational relaxation rates. The initial gas mixture used was $1 \text{ H}_{2^{15}} \text{ SF}_{6}$ at 120 Torr and 300°K. Mirror reflectivities of the optical cavity were taken to be 1.0 and 0.8, and the gain length was 50.8 cm. The total atomic fluorine introduced into the mixture was 5.6% of the SF₆ concentration. The results are given in Table 2.2 of four selected cases: (1) rotational equilibrium maintained; (2) the rotational relaxation time constant approximately the inverse of the gas kinetic collision frequency; (3) rotational relaxation modeled at 10% of the rate in case (2); and (4) rotational relaxation modeled at 1% of the second case.

The first and second cases have very similar results. The relaxation time for the second case is comparable to the time required for light to traverse the length of the active medium. At slower rotational relaxation times, the populations in the various J-states do not contribute instantaneously to the lasing in any given line. This has a two-fold consequence: (1) Energy is extracted less rapidly, which allows more time for the deactivation mechanisms

Model Predictions of effect of rotational relaxation rate on laser output 2. 2. Table

| iper e R. ire i lie di ite i | risn Or 1 st | Energy | J/cc |) Indy | Time, µ | Isec |
|--|--------------------|---------|---------|-----------|-------------|-------|
| A_ | E10 | E21 | E32 | E | t i | t1/2 |
| Rotational Equilibrium | 0.00590 | 0.00723 | 0.00185 | 0.0150 | 0.320 | 0.130 |
| $2 \times 10^{-9} \text{ T}^{-1/2}$ | 0.00593 | 0.00723 | 0.00185 | 0.0150 | 0.330 (est) | 0.140 |
| $2 \times 10^{-8} \text{ T}^{-1/2}$ | 0.00579 | 0,00689 | 0.00169 | 0.0144 | 0.364 | 0.140 |
| $2 \times 10^{-7} \text{ T}^{-1/2}$ | 0.00468 | 0.00581 | 0.00110 | 0.0116 | 0.390 | 0.135 |

to act. This results in a more uniform distribution of output energy among the lasing transitions of a given band and a net decrease of the total pulse energy (Figure 2, 7). (2) Since the higher J-state populations are not instantaneously coupled to the populations of the lasing transitions, these higher J-transitions reach threshold earlier and multiline lasing becomes more prevalent. Lasing on higher J levels also increases as τ_p increases (Figure 2.8). The decrease in the predicted total laser output as a result of rotational nonequilibrium effects was expected. Since previous model predictions have been significantly higher than actual experimental values, inclusion of this effect is helpful in achieving agreement between theory and experiment. This, however, is not necessarily the only source of discrepancy between theory and experiment. * In Figure 2.9, the third case is compared with Lyman's model and the experimental result from Beattie et al. 38 This result indicates that even with rotational relaxation, model predictions of pulse output are still higher than the experimental values. ** Lyman used for his calculations essentially the initial rate coefficients compiled by Cohen in 1971. For the calculations of this study, rate coefficients reflecting more recent experimental data were used. 33

One of the most significant results of the incorporation of rotational relaxation into the model is the appearance of multiline lasing (compare Figures 2.8.a, 2.8.b, and 2.8.c). The overlapping of

See Reference 26, where the discrepancy was ascribed mostly to parasitics.

^{**} The data in Figure 2.9 were taken from Figure 7 of Reference 27. Note that the calculations in Reference 27 were made with $R_L = R_{c} = 1$.



Figure 2.7. Comparison of power histories for three different rotational relaxation rates.



Figure 2.8. Power histories for all transitions in 2-1 band for three different rotational relaxation rates. (a) rotational equilibrium, (b) $A_{T} = 2 \times 10^{-8} T^{-1/2}$, (c) $A_{T} = 2 \times 10^{-7} T^{-1/2}$.



Figure 2.9. Comparison of power histories as determined by present model and by Lyman's model with experimental result of Beatie et al.³⁸ The present model result has been smoothed for this comparison.

the transitions in a given band has always been seen experimentally.^{30,32} Time-resolved spectra that follow a J-shifting sequence similar to that shown in Figure 2.8 are reported in References 31 and 32. However, the spectrum found by Suchard et al.^{29,30} shows significant departure from the sequential J-shift pattern. One possible explanation of their result was thought to be the non-Boltzmann product distribution of the pumping reactions. For these calculations, a Boltzmann distribution was not assumed, but the results still show a consistent J-shifting pattern. The results, however, are expected to be sensitive to cavity losses. A second calculation was made for the third case, with an assumed Boltzmann distribution among the rotational states of the product molecule HF(v), in order to check the significance of the role of preferential pumping. The results in Table 2.3 show that, for the gas mixture and the cavity condition considered, the effect is small. Preferential pumping resulted mainly in a slight increase in output energy for the higher J-transitions.

One added advantage of modeling rotational relaxation is that the model has the capability of estimating performance in lineselected modes. In Table 2.3, a comparison is made of the laser performance for various modes of operation. It is apparent that maximum output energy is obtained from a laser where all transitions are allowed to reach threshold and lase. The effect of cascading is also evident. The sum of the pulse output from the three single-line calculations, i.e., $P_1(8)$, $P_2(7)$, and $P_3(6)$, is only 65% of the output for the case with these three transitions operating in a cascading manner. The "off-J" cases, i.e., $P_1(9)$, Table 2.3. Model predictions for a representative rotational relaxation rate^a

| Onersting Mode | | Energy, | J/cc | | Time, | рвес |
|--|-------------------|-------------------|-----------------|---------|-------|------------------|
| Operating more | $\mathbf{E_{10}}$ | \mathbf{E}_{21} | E ₃₂ | Е | t1 | t _{1/2} |
| Multiline | 0.00579 | 0.00689 | 0.00169 | 0.0144 | 0.364 | 0.140 |
| P ₁ (8) Single Line | 0.00287 | 0 | 0 | 0.00287 | 0.235 | 0.120 |
| P ₂ (7) Single Line | 0 | 0.00425 | 0 | 0.00425 | 0,288 | 0.143 |
| P ₃ (6) Single Line | 0 | 0 | 0.00001 | 0.00001 | 0.030 | 0.015 |
| P ₁ (8), P ₂ (7), P ₃ (6) | 0.00435 | 0.00542 | 0.00119 | 0.0110 | 0,265 | 0.116 |
| P ₁ (9), P ₂ (7), P ₃ (5) | 0.00342 | 0.00476 | 0.00032 | 0.0085 | 0.275 | 0.150 |
| Multiline With No Preferential Pumping | 0.00562 | 0.00676 | 0.00176 | 0.0142 | 0.355 | 0.140 |

 ${}^{a}A_{T} = 2 \times 10^{-8} \text{ T}^{-1/2}$

 $P_2(7)$, and $P_3(5)$, show a decrease in output energy when compared with the cascading case.

2.4 Summary

Rate-equation models that graphically illustrate the effect of gain fluctuation and rotational nonequilibrium on pulsed HF laser performance are presented. In the present investigation, it was determined that incorporation of these effects into chemical-laser models is essential for the accurate investigation of the spectral content in the laser pulse. Examination of the effect of line-selected operation on pulse energy indicates that considerable care in line selection must be made to avoid large energy losses and that a model similar to the one developed in this investigation will be helpful in selecting transitions for beam propagation.

3. EFFECT OF CAVITY LOSSES ON PERFORMANCE OF THE SF₆-H₂ PULSED CHEMICAL LASER: THEORY AND EXPERIMENT

3.1 Introduction

Because of the potential for high performance, the reaction of hydrogen and the halogens have been used widely in the production of active species for chemical lasers. $^{13,38,53-55}$ Of these, the HF and DF systems have been studied most often because of the potential for developing lasers with high specific power densities through the the use of a chemical chain reaction. In an electrical discharge, SF₆ will provide the F atoms for the reaction

$$F + H_2 \rightarrow HF(v) + H$$
 (3.1)

The vibrationally excited HF can then be used as the laser medium. The SF_6-H_2 laser has proved to be a valuable tool in the examination of mechanisms in HF and DF lasers. With this laser, the extra expense and complications of handling a potentially dangerous gas are avoided, while sacrificing little in the study and interpretation of the mechanisms.

Several researchers $^{56-59}$ have investigated the effect of the use of different initiation techniques to increase the efficiency of the SF_6-H_2 chemical laser. However, with the exception of the measurements of the variation of laser output with output compling made by

Jones,⁶⁰ no formal attempt has been made to systematically identify the role of cavity losses in the performance of this device. The results of such an investigation are presented here, where the experimental data were obtained using a transverse pin-discharge laser, and the theoretical predictions were made from the computer model given in Chapter 2, which includes in its computations the effects of rotational nonequilibrium.

3.2 Experimental Details

Figure 3.1 is a schematic diagram of the pulsed SF_6-H_2 laser facility used in this investigation. The gas mixture is contained in two 1-in. i.d., 49-1/2 in. long, lucite tubes placed end to end. Both ends of the tubes are sealed by CaF₂ flats mounted at the Brewster angle for 2.8-µm transmission. The electrode assembly is made up of 338 resistor (470 Ω) pin-pairs set transverse to the laser axis and mounted on the lucite tubes in a double helical configuration. The interelectrode gap is set at 2.08 cm. The optical cavity is formed external to the tubes and consists of a 7.0-m radius, concave spherical, dielectric-coated (silicon substrate) for a nominal 99% reflectivity at 2.5 to 3.5 μ m and a flat-output coupler, dielectriccoated (silicon substrate) for 95 + 1-5% reflectivity at 2.5 to 3.5 μ m. Pulsed high voltage is obtained by means of a 5400 pF energy storage capacitor, the voltage of which is applied across the electrodes by triggering a spark gap (EG&G, Model 14B). The trigger circuit used is shown in Figure 3.2.

Figure 3.3 is a schematic diagram of the gas-handling system. The gases (SF₆, H_2 , and He) were research grade (99.99% pure) supplied by Matheson and were used without further purification. The flow rates were controlled and measured with Matheson



Figure 3.1. Michigan State University SF₆-H₂ pulsed chemical laser facility.



Figure 3.2. Circuit used to trigger spark gap for application of pulsed high-voltage across discharge electrodes.



Figure 3.3. Gas-handling system that provided calibrated gas mixtures for SF₆-H₂ laser.

needle valves and flownmeters. Pressures were monitored on Heise Bourdon tube gauges. A mechanical pump (Kinney) is used to maintain a continuous gas flow through the laser and provide for operation over a range of pressures.

Pulse output is focused by a 2-in.-diameter gold-coated concave spherical mirror of 45.2-cm radius of curvature into a 0.5-m monochrometer (McKee-Pederson) equipped with a 295 line/mm grating blazed at 2.8 µm. Radiation emerging from the monochromator is detected by a Au:Ge photodiode detector (Raytheon) operated at 77°K and displayed on a fast-rise (1.2 nsec) oscilloscope (Tektronix 485). Screens were placed before the detector to avoid saturation.

Because of the potential high gain of the HF system, under some operating conditions, relatively strong output has been measured from laser cavities with the mirrors removed. $^{60-62}$ This phenomenon is known as superradiance. Except for performance studies, typical runs in the present experiments were made at 33 Torr, in a 1 SF₆:1 H₂:10 He gas composition, and at 30-kV discharge voltage. The power output decreased by two orders of magnitude with the mirrors removed; therefore, superradiance did not affect the measurements.

At the beginning of each run, the laser chamber is pumpeddown to check for possible leaks and to re-zero the pressure gauges. The pulse repetition rate is limited by the time required to recharge the capacitors and the exchange rate of the gases within the cavity. For best repeatability, approximately 15 sec was allowed between shots. A comparison of the output for a single shot and ten superposed shots showed that, except for some erratic fringes, the pulses were repeatable.

The experimental setup is shown schematically in Figure 3.4. A scheme is desired whereby losses may be introduced into the cavity without otherwise altering the existing optical configuration (as may happen, for example, by changing the output coupler and realigning). An effective variation of the output coupling is accomplished by inserting a CaF₂ attenuator into the optical cavity, as is shown in the Figure 3.4. The threshold gain (α_{thr}) is then given by the equation

$$R_{o}R_{L}t^{2}e^{(2\alpha_{thr}L)} = 1$$
 (3.2)

where R_0 and R_L are the reflectivities of the output coupler and total reflector, respectively, t is the transmissivity of the attenuator, and L is the gain length in the medium. Since t is a function of the angular position of the CaF₂ attenuator, a continuous range of α_{thr} may be obtained by varying that angle. In addition to the attenuator, a CaF₂ compensator is placed outside the optical cavity in the path of the output radiation to compensate for the vertical displacement of the laser output resulting from the attenuator. An iris is inserted in the optical cavity to increase the threshold for parasitics.⁶⁰ It also functions as a mode-control device. The iris opening is decreased until further decreases result only in a monotonic decrease in output Power, indicating dominance by the TEM₀₀ mode. To ensure a more accurate determination of the angular position of the attenuator, this angle is measured by the calibrated position of a He-Ne beam



Figure 3.4. Experimental setup for introduction of variable loss into laser cavity.

reflected from a mirror affixed to the attenuator (Figure 3.4). A similar arrangement is used for the compensator.

3.3 Computer Simulation

The computer code is described in Chapter 2. The predicted output lasing power per unit volume is, from Equation (2.9),

$$P_{L}(t) = \sum_{v,J} hc N_{A} \alpha_{thr} \omega_{c}(v,J) f(v,J)$$
(3.3)

where $\omega_c(v, J)$ is the wave number of the $v + 1 \rightarrow v$ transition with lower level J, and f(v, J) is the lasing flux on the same transition, α_{thr} is the threshold gain defined by

$$\alpha_{\rm thr} = -\frac{1}{2L} \ln({\rm R'_o R_L}) \tag{3.4}$$

where L is the length of the active medium and R'_{o} and R_{L} are the effective mirror reflectivities.

The laser power $P_L(t)$, in Equation (3.3), is the sum from both **mirrors** of the cavity. The output intensity extracted from mirror **R**²² is ²²

$$P'_{o} = \frac{(1 - R'_{o})}{\left[1 + (R'_{o}/R_{L})^{1/2}\right] \left[1 - (R'_{o}R_{L})^{1/2}\right]} P_{L}(t)$$
(3.5)

Initial conditions and model parameters are determined to reflect conditions of the experiments. The electrical-dischargeinitiated laser used in the present investigation produced columns of nearly uniform plasma orthogonal to the laser axis. Since diffusion is negligible during the pulse, the active region of the laser may be approximated as homogeneous. The active medium length is taken to be the sum of the diameters of these columns and is estimated to be 169 cm. Various types of losses within the cavity are lumped with the 99% reflecting spherical mirror for an estimated value $R_L = 0.95$. The output coupler is taken as $R'_0 = R_0 \times t^2(\theta)$, where $t(\theta)$ is the transmittance of the CaF₂ attenuator set at angle θ to the laser axis and $R_0 = 0.95$ is the true reflectivity of the output coupler. The power extracted from R'_0 , as given by Equation (3.5), includes losses resulting from reflection from the attenuator out of the optical cavity, as well as actual power passing through R_0 . This loss can be corrected for by means of Equation (E.6), Appendix E, to obtain **finally**

$$P_{o}(t) = \frac{t(1 - R_{o}')(1 - R_{o})P_{L}(t)}{\left[1 + (R_{o}'/R_{L})^{1/2}\right]\left[1 - (R_{o}'R_{L})^{1/2}\right]\left[1 - R_{o}'\right]} \quad (3.6)$$

Electric discharge initiation, i.e., abstraction of F atoms $\mathbf{from} SF_{k}$, is approximated by the relation

$$\frac{dN_{\rm F}}{dt} = C P_{\rm I}(t) N_{\rm SF_6}$$
(3.7)

where $P_{I}(t)$ is the normalized discharge power profile and C serves as a parameter to couple the experimental results to theory. The **Parameter** C is determined by matching the computed pulse duration and the time that it takes for the laser to reach threshold with the **measured** times for a selected case. Since the laser output was attenuated, comparisons of theory and experiment are accomplished by matching the outputs at a selected reference point.

3.4 Results and Discussion

Typical oscilloscope traces for the discharge current and the total laser output along with the corresponding predicted laser pulse are shown in Figure 3.5. The discharge current behaved like a damped oscillator with a one-half period (FWHM) of 0.26 μ sec. The resulting laser pulse was of similar duration (0.24 μ sec, FWHM), while the "tail" of the pulse was considerably lengthened by the second half-period of the discharge current. Calculations from the model showed that, near this level of initiation, i.e., F/SF₆ = 0.005, the laser pulse shape is quite sensitive to that of the discharge current.

Figure 3.5 shows that the predicted pulse shape compares very well with that observed on the oscilloscope. The "knee" at the beginning of the pulse is due to lasing on the 2-1 band, which has the highest pumping rate. This lasing populated the upper level of the 1-O band and depleted the lower level of the 3-2 band, complementing the pumping on those levels. Thus, gain on the 3-2 and 1-0 bands rose rapidly and lasing commenced on all bands, which caused the ab rupt rise in the observed output pulse. Thereafter, lasing was sustained by the fast-pumping reaction. Pulse termination resulted when pumping subsided and lasing and collisional deactivation have depleted the population inversion.

Model predictions of total laser output and the corresponding **b**served output are plotted in Figure 3.6 as a function of cavity **losses.** The theoretical values were computed from Equation (3.6).

- Figure 3.5.a. Typical oscilloscope trace of discharge current during laser initiation.
 - b. Oscilloscope trace of laser output for $1 H_2:1 SF_6:10$ He mixture at 50 Torr. Attenuator angle θ set at 0 deg.
 - c. Laser output predicted by present model at same gas mixture and cavity condition. The predicted time to threshold, pulse width, and pulse shape are similar to that in (b).



Figure 3.5

In conjunction with Equation (3.4), $R'_{o}R_{L}$ is a measure of the sum of the cavity losses, which are in the form of laser output as well as transmission through the spherical mirror, reflection from the attenuator, and other extraneous losses. Three cases are shown: (1) 0.2 H_2 :1 SF₆:10 He at 33 Torr, (2) 1 H_2 :1 SF₆:10 He at 33 Torr, and (3) 1 H₂:1 SF₆:10 He at 50 Torr. The lower gain cases, (1) and (2), were selected to avoid possible complications resulting from parasitic oscillations or superradiance. When agreement between theory and experiment was good, a higher gain case, (3), was run. In Figure 3.6, the curves represent model predictions of laser output as a function of cavity threshold. The vertical bars represent the scatter in the measured data. In general, the calculated and observed quantities agree rather well. Both indicate a decrease in **La**ser output with increasing cavity loss, i.e., decreasing $R'_{O}R_{L}$. The experimental data, however, indicate a somewhat smaller slope $f \circ r$ the curve than that predicted, especially in the region of higher $1 \circ s$ s. The higher loss conditions correspond to smaller attenuator angles (approximately 0 to 20 deg).

It was demonstrated in Chapter 2 that rotational relaxation and rotational nonequilibrium play a significant role in the character and Performance of the HF chemical laser. Since the rotational relaxation rates are generally unknown, it is appropriate that an examination be made of the sensitivity of the present calculations to these rates. The rotational relaxation rate was increased by an order of Magnitude from the gas kinetic frequency to ten times the gas kinetic collision frequency between HF molecules and all collision partners. The results indicate that there is no extensive change for this case.



Figure 3.6. Effect of cavity losses on total laser output for three gas mixtures. (a) 0.2 H₂:1 SF6:10 He at 33 Torr, (b) 1 H₂:1 SF6:10 He at 33 Torr, (c) $1 H_2$: 1 SF6:10 He at 50 Torr

Because of the rotational relaxation provision in the model, it is well suited for making calculations of laser operation in the lineselected mode. The experiment was repeated for the laser operating on a single line. The transitions $P_1(4)$ and $P_2(3)$ were selected, since these were observed to be among the strongest lines in the pulse output spectra. The results for the $P_1(4)$ and $P_2(3)$ comparisons are presented in Figures 3.7.a and 3.7.b, respectively. The discrepancy between theory and experiment is more severe in the $P_2(3)$ case. This behavior is not expected from considerations of the kinetic mechanisms involved, and may be partially due to the fact that mode structure and diffraction losses were not incorporated into the model. Further study is necessary to clarify this point.

Note that the value assigned to R_L is somewhat arbitrary. Fortunately, calculations indicate that the shapes of these theoretical curves are not sensitive to that value. If, for example, R_L were assigned the value 0.90 instead of the 0.95 presently used, the maximum change in predicted pulse energy in Figures 3.7.a and 3.7.b for any given $R'_O R_L$, is less than 2.5%, which is significantly smaller than the experimental data scatter.

The rotational-relaxation rate is an important factor in determining the rate at which the population inversion of a given transition will be restored or maintained following laser action on that transition. It is expected that, with the laser operating in the single-line mode, as the rotational relaxation rate is increased, more energy would be extracted. This was verified by calculations. As in the multiline case, the rotational-relaxation rate was increased from gas kinetic to ten times gas kinetic with the laser operating in the


Figure 3.7. Effect of cavity losses on output of laser operating in single-line mode for two selected transitions. (a) P₁(4), (b) P₂(3). Note significant loss in useful laser output that resulted from parasitic oscillations, as shown in (a)

single-line mode on the $P_2(3)$ transition. The laser output increased by approximately 6% for various values of $R'_{O}R_{L}$ but had very little effect on the overall shape of the theoretical curve presented in Figure 3.7.b.

The U-shaped curve (Figure 3.7.a) represents an interesting example of off-axis parasitics that resulted in a reduction of laser output. Here, in the changing of the effective reflectivity of the output coupling, the attenuator was turned in the counterclockwise direction. When the normal to the attenuator was approximately 20 to 40 deg from the laser axis, the detector showed an abrupt drop in laser power. The CaF₂ attenuator had apparently coupled itself to the walls of the laser chamber and produced off-axis oscillations. Similar results were observed for the $P_2(3)$ and multiline cases at these angles, although the power reductions were not as large. In the $P_1(4)$ case, lasing on the 1-0 band, which depleted the v = 1 level, and the fact that the pumping to the v = 2 level is at least twice as fast as that to any other vibrational level, lead to large population inversions in the 2-1 band transitions. Since lasing on those transitions was suppressed in this mode, parasitics were expected. Parasitic oscillations were not evident when the attenuator was turned in the clockwise direction, with all possible extraneous reflecting surfaces outside the laser chamber covered by a thin layer of sponge.

The results shown in Figures 3.6 and 3.7 illustrate the importance of "small" cavity losses that are often neglected in the design of optical cavities. At the angles of maximum attenuation the CaF_2 attenuator used in these experiments has typical transmission coefficients greater than 93%, and the power reduction, in some cases, is more than 50%. When the extraneous losses in the cavity become comparable to the output coupling, large power reductions will result. Thus, as the Q of the cavity is increased, the problem progressively worsens. One possible source of such losses in the gas laser is the Brewster window. While this window theoretically has a transmissivity of 100% for radiation with polarization parallel to the plane of incidence, it may still be an important source of losses for some laser systems. (In high power lasers, there may be window or mirror, or both, damage after a few shots.) In addition to losses resulting from scattering and absorption, the windows could serve as couplers for off-axis parasitic oscillations.

Given the reasonably good agreement between theory and experiment, one is encouraged to proceed with some confidence in the model. Model calculations of the effect of threshold condition on the laser pulse energy are given in Figure 3.8. A more typical, higher gain gas mixture was selected, and a wider range for α_{thr} was used. The gas composition was 100 Torr of SF₆ and 20 Torr of H₂. Three representative cases are presented: (1) total pulse energy; (2) P₂(3) in the single line mode; and (3) P₃(6), P₂(7), and P₁(8), in the cascade mode. For the DF laser, these three lines in the cascade are known to have good transmission coefficients through the atmosphere. * The resultant curves show the expected profile: At high threshold, lasing is delayed and sporadic and a large portion of the pumping energy is lost through deactivation. At low threshold, energy is not extracted

^{*}D. J. Spencer, The Aerospace Corporation, private communication, September 1974.

Figure 3.8. Model calculations of the effect of cavity threshold on pulse energy for a 1 H2:5 SF₆ mixture at 120 Torr, with laser operating in three different modes. (a) multi-line mode; (b) single-line mode on P₂(3) transition; (c) cascade mode of three transitions, P₃(6), P₂(7), and P₁(8)



Figure 3.8

efficiently from the optical cavity, although intensities within the cavity reach relatively high levels. This condition is also the most susceptible to power reduction resulting from "minor" cavity losses. The optimum performance lies between these two extremes.

3.5 Summary

A theoretical and experimental investigation was conducted to assess the role of cavity losses in the performance of the pulsed chemical laser in the single-line and the multiline modes. Although the investigation was carried out with the SF_6 -H₂ laser, the results are believed to be of more general validity. It was found that losses within the optical cavity, of as little as 5%, typical of many lasers, can easily result in a 30% or more reduction in power output. This problem becomes especially acute for high-Q cavities. In addition, model predictions are presented that graphically illustrate the effect of cavity threshold on laser output. This includes, for the first time, predictions of performance in the single-line and cascading modes.

4. SUMMARY AND CONCLUSIONS

Computer models are presented that simulate the performance of the $H_2 + F_2$ chain reaction and the SF_6-H_2 pulsed chemical lasers. Rate equations are used to represent the chemical kinetic and stimulated emission processes occurring in a representative unit volume within a Fabry-Perot cavity. All processes are assumed uniform throughout the cavity. Lasing is permitted on all lines in the vibrational-rotational bands that reach threshold and may respond to gain fluctuations during the lasing period. Rotational relaxation is incorporated into the model of the SF₆-H₂ laser to study the effect of rotational nonequilibrium on the laser performance. The individual rotational level populations are determined from the solution of rate equations. Relaxation of the rotational population is accomplished by the assumption of a characteristic rotational-relaxation time similar to the model of Schappert³⁴ for CO₂. With the rotational populations of the first four vibrational levels identified, the effects of single-line operation can be examined.

Comparisons of the predictions of this model with that of the constant-gain model illustrated the unique features of the present model. The present formulation facilitated the determination of the time evolution of gain, intensity, and species concentration. Interaction of gain and intensity before and during lasing was observed.

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Contrary to the constant-gain model, lasing did not commence upon gain reaching threshold. The growth of intensity was sufficiently slow such that lasing effectively began only after the gain was well above threshold. This usually resulted in a large initial spike in the intensity, which could be a potential source of damage to windows and mirrors in high power lasers.

In addition to the prediction of transients and relaxation oscillations seen experimentally, this model demonstrated greater sensitivity to nonlinear mechanisms such as vibrational-vibrational (VV) deactivation. This resulted in the prediction of shorter pulses in the laser output.

Calculations from the model showed that the assumption of a Boltzmann distribution among the rotational-state populations precluded extensive multiline-lasing and that such multiline lasing became prevalent only when rotational-relaxation effects were considered. Rotational relaxation also accounted for a decrease in predicted laser output; this prediction is more consistent with experiment. The modeling of rotational relaxation permitted, for the first time, an evaluation of the performance of a chemical laser when operating in the line-selected mode. Calculations were made of the SF₆-H₂ laser oscillating on a single line for each of the three transitions P₁(8), P₂(7), and P₃(6). The sum of the pulse output from the three single-line calculations is only 65% of the output for the case with these three transitions operating in a cascading manner. For the gas mixture and cavity conditions considered, the effect of preferential pumping on rotational nonequilibrium and laser performance was small. It resulted mainly in a slight increase in output energy for the higher J transitions. This behavior, however, may be sensitive to cavity threshold.

This model was used in a theoretical and experimental investigation of the effect of cavity losses on the performance of a SF_6-H_2 laser. The experimental data are expected to provide a test of the validity of the model's predictions and assumptions. At low levels of initiation, as with the present case, the laser pulse shape is sensitive to that of the discharge current. The predicted pulse shape and pulse width are in good agreement with experimental observations. Good agreement between theory and experiment is also found in the prediction of pulse output variation with cavity losses, for the laser operating on the single transitions $P_1(4)$ and $P_2(3)$, as well as in the multiline mode. Although not modeled, parasitic oscillations was shown to be an important consideration in the investigation of laser performance. Under some operating conditions, it could lead to significant losses in the useful laser output. Laser performance as a function of cavity threshold is also of interest. Calculations of the effect of output coupling are presented for the cases of multiline operation, single-line operation on the $P_2(3)$ transition, and the cascade of the three transitions $P_3(6)$, $P_2(7)$, and $P_1(8)$.

The model has demonstrated remarkably good agreement with experimental observations. One can conclude that there are no gross inaccuracies in the chemical kinetic or radiative formulation of the model. As shown in Chapter 3, however, there are factors such as cavity losses and parasitic oscillations which exist in real

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lasers that are unaccounted for, but which could have appreciable effect on the laser character. These factors obviously are not easily modeled.

There are other phenomena that are not modeled which exist within most lasers: Mode competition and mode beating, intensity distribution transverse to the laser axis, medium inhomogeneity, temperature gradients, acoustic effects, interaction with the walls. and plasma kinetics in the case of electrical discharge initiation. Attempts were made in the present experiments to eliminate or minimize the effects of some of these unknown inputs. An iris was used to maintain dominance of the TEM ____ mode in the radiation field, thus mode competition is minimized. The particular configuration selected for this laser resulted in a high-gain path along the axis of the laser away from the walls. Thus, in the time scale of the laser pulse, interaction with the wall is highly unlikely. The effect of medium inhomogeneity or temperature gradients have not been studied. These could result in irregularities along the gain path and distortions in the radiation field, but the net effect may average out along the laser axis and result in only minor alterations of the laser output.

The lack of plasma chemistry in the model appeared to be a serious drawback in these experiments. Initiation through electrical discharge proceeds through the creation of a partially ionized plasma that includes in its composition excited and metastable species as well as ion-electron pairs and neutral particles. Production of F atoms necessary for the pumping reaction is the result of complex processes within the plasma such as charge transfer, Penning

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ionization, recombination, detachment, and attachment. The model presented here, however, incorporates no plasma kinetics. Nevertheless, since only a small fraction of the gas is ionized (typically less than 5%; in this case, less then 2%), the effect of these charged particles on the neutral chemistry and the associated model predictions is expected to be minimal. The most important contribution of the plasma kinetics is F-atom production, which was found by Lyman to be roughly proportional to the input power. This fact was incorporated into the model empirically.

The rotational-relaxation process modeled in this investigation represents only an initial step in a rapidly developing area of active research. Recognition of the importance of the role of rotational nonequilibrium and rotational relaxation in the behavior of chemical lasers has led to several recent studies, both theoretical⁶³⁻⁶⁵ and experimental. ^{*} While the formulation adopted in this work has been valuable in the prediction of broad effects of rotational relaxation and in providing physical insight into the problem, the rotational relaxation rates now being measured will permit a more accurate study to be made of these phenomena through a careful model of the detailed collisional dynamics involved in the processes. To be complete, this model should include the effects of R-branch and J-J lasing. However, the increased computational complexities resulting from these additions make this proposition impractical for the present day generation of computers. Further experimental verifications of the model predictions are desirable. Experiments such as small-signal-gain probing and Raman scattering would provide valuable data on the species concentrations within the laser medium, and side-arm chemiluminescence could be used to verify the predicted high-gain overshoots. APPENDICES

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APPENDIX A

RATE COEFFICIENTS FOR $H_2 + F_2$ CHEMICAL LASER

APPENDIX A

RATE COEFFICIENTS FOR $H_2 + F_2$ CHEMICAL LASER

The chemical kinetic model used for the rate-equation solution has been suggested by $Cohen^{33}$ and is shown in Table A.1. Rate coefficients k and k- designate forward and backward rates, respectively. For each reaction, the missing rate coefficient is determined from the equilibrium constant.

| Reaction No. | Reaction | Rate Coefficient, cc/mol-sec | M, v |
|------------------------------|---|---|--|
| ta ^b | $F + H_2(0) = HF(1) + H$ | $k_{1a} = 2.6 \times 10^{13-1.6/\theta}$ | |
| ib | $F + H_2(0) = HF(2) + H$ | $k_{1b} = 8.8 \times 10^{13-1.6/9}$ | |
| tc | $F + H_2(0) = HF(3) + H$ | $k_{1c} = 4.4 \times 10^{13-1.6/\theta}$ | |
| tđ | $F + H_2(0) = HF(4) + H$ | $k_{-1d} = 7.4 \times 10^{12-0.50/0}$ | |
| 1e | $F + H_2(0) = HF(5) + H$ | $k_{-1e} = 1.1 \times 10^{13-0.51/\theta}$ | |
| 1 f | $F + H_2(0) = HF(6) + H$ | $k_{-1f} = 1.9 \times 10^{13-0.56/\Theta}$ | |
| 2a | $H + F_2 = HF(0) + F$ | $k_{2a} = 1.1 \times 10^{12-2.4/0}$ | |
| 2Ъ | $H + F_2 = HF(1) + F$ | $k_{2b} = 2.5 \times 10^{12-2.4/\theta}$ | |
| 2 c | $H + F_2 = HF(2) + F$ | $k_{2c} = 3.5 \times 10^{12-2.4/\theta}$ | |
| 2d | $H + F_2 = HF(3) + F$ | $k_{2d} = 3.6 \times 10^{12-2.4/0}$ | |
| 2e | $H + F_2 = HF(4) + F$ | $k_{2e} = 1.6 \times 10^{13-2.4/\Theta}$ | |
| Zſ | $H + F_2 = HF(5) + F$ | $k_{2f} = 3.6 \times 10^{13-2.4/\Theta}$ | |
| 2g | $H + F_2 = HF(6) + F$ | $k_{2g} = 4.8 \times 10^{13-2.4/0}$ | |
| 2h | $H + F_2 = HF(7) + F$ | $k_{2h} = 5.5 \times 10^{12-2.4/\theta}$ | |
| Zi | $H + F_2 = HF(8) + F$ | $k_{2i} = 2.5 \times 10^{12-2.4/0}$ | |
| 3a _v ^c | $HF(v) + M_{1} = HF(v - 1) + M_{1}$ | $k_{3a_v} = v(10^{14.0} \text{ T}^{-0.8} + 10^{0.4} \text{ T}^{3.5})$ | $M_1 = HF, v = 1 \cdot \cdot \cdot 8$ |
| 36 ₁ | $HF(1) + M_2 = HF(0) + M_2$ | $k_{3b_1} = 1.5 \times 10^{10-1.1/\theta} T$ | M ₂ = F |
| 3 ^b 2 | $HF(2) + M_2 = HF(1) + M_2$ | $k_{3b_2} = 1.5 \times 10^{10-0.5/\theta} T$ | |
| 3hv | $HF(v) + M_2 = HF(v - 1) + M_2$ | $k_{3b_{v}} = 1.5 \times 10^{10} \text{ T}$ | v = 3 · · · 8 |
| 3c _v | $HF(v) + M_4 = HF(v - 1) + M_4$ | $k_{3c_v} = (8 \times 10^{-4} \text{ T}^4)v$ | $M_4 = Ar, F_2, SF_6; v = 1 \cdot \cdot \cdot$ |
| 3d _v | $HF(v) + M_5 = HF(v - 1) + M_5$ | $k_{3d} = v(8.7 \times 10^{-7} \text{ T}^5)$ | M ₅ = He v = 1 · · · 8 |
| 3e _v | $HF(v) + M_{6} = HF(v') + M_{6}$ | $k_{3e_v} = 1.8 \times 10^{13-0.7/9}$ | $M_6 = H v = 1 \cdot \cdot \cdot \cdot 8, \ v' < v$ |
| 3f _v | $HF(v) + M_7 = HF(v - 1) + M_7$ | $k_{3f_{11}} = v(1 \times 10^5 T^2)$ | $M_7 = H_2 v = 1 \cdot \cdot \cdot 8$ |
| 4a | HF(v) + HF(v) = HF(v - 1) + HF(v + 1) | $k_{4a} = 1.5 \times 10^{12} \text{ T}^{1/2}$ | v = 1 · · · 7 |
| 4 b | HF(v) + HF(v + 1) = HF(v - 1) + HF(v + 2) | $k_{4b} = 0.5k_{4a}$ | v = 1 · · · 6 |
| 4c | HF(v) + HF(v + 2) = HF(v - 1) + HF(v + 3) | $k_{4c} = 0.25k_{4a}$ | v = 1 · · · 5 |
| 4d | HF(v) + HF(v + 3) = HF(v - 1) + HF(v + 4) | $k_{4d} = 0.125k_{4a}$ | v = 1 · · · 4 |
| 5a | $HF(0) + H_2(1) = HF(1) + H_2(0)$ | $k_{5a} = 9 \times 10^{11}$ | |
| 5Ъ | $HF(1) + H_2(1) = HF(2) + H_2(0)$ | $k_{5b} = 2.9 \times 10^{12}$ | |
| 5c | $HF(2) + H_2(1) = HF(3) + H_2(0)$ | $k_{5c} = 9 \times 10^{12}$ | |
| 5d | $HF(3) + H_2(1) = HF(4) + H_2(0)$ | $k_{5d} = 2 \times 10^{13}$ | |
| 5e | $HF(0) + H_2(2) = HF(1) + H_2(1)$ | k _{5e} = k _{5a} | |
| 5 L | $HF(1) + H_2(2) = HF(2) + H_2(1)$ | k _{5f} = k _{5b} | |
| 6 a _v | $H_2(v) + M_8 = H_2(v - 1) + M_8$ | $k_{6a_v} = v(2.5 \times 10^{-4}) T^{4.3}$ | v = 1, 2 M ₈ = all except H, H ₂ |
| ^{7b} v | $H_2(v) + M_9 = H_2(v - 1) + M_9$ | $k_{7b_v} = v(10^{-3} T^{4,3})$ | $v = 1, 2 M_9 = H, H_2$ |

Table A.1. Rate coefficients for $H_2 + F_2$ chemical laser^a

^aNote dissociation-recombination reactions have been neglected.

 $b_{\theta} = 4.575 \text{ T}/1000 \text{ kcal/mol}$

^cv = vibrational level; M = collision partner

DERIVATION OF THE RADIATIVE TRANSFER EQUATION

APPENDIX B

APPENDIX B

DERIVATION OF THE RADIATIVE TRANSFER EQUATION

Let

$$N_{ij} = HF(v + 1, J - 1)$$
 (B.1.a)

$$N_1 = HF(v, J) \tag{B.1.b}$$

where N_u and N_l are the concentrations in mol cm⁻³ of, respectively, the upper and lower states of the transition. Following Gilles and Vincenti⁶⁶ and Emanuel,¹¹ the transfer equation for radiation of intensity (I_v) passing through the active medium in the x direction is

$$\frac{dI_{\nu}}{dx} = h\nu N_{A}\phi(\nu) [N_{u}A_{ul} + (N_{u}B_{ul} - N_{l}B_{lu})I_{\nu}]$$
(B.2)

where N_A is the Avagadro's number; A_{ul} , B_{ul} , and B_{lu} are Einstein coefficients defined in terms of the intensity per unit solid angle; A_{ul} is the coefficient for spontaneous emission; B_{ul} and B_{lu} are the coefficients for stimulated emission and absorption, respectively; and $\phi(\nu)$ is the line-shape function normalized according to

$$\int_{0}^{\infty} \phi(\nu) d\nu = 1 \qquad (B.3)$$

Equilibrium considerations and detailed balancing require that⁶⁷

$$A_{ul} = 2h\nu^3 \left(\frac{B_{ul}}{c^2}\right) \qquad B_{ul} = \left(\frac{q_l}{q_u}\right) B_{lu} \qquad (B.4)$$

where q represents the degeneracy of the level. Thus, Equation (B.2) is written

$$\frac{\mathrm{dI}_{\nu}}{\mathrm{dx}} = h\nu N_{A}\phi(\nu) \left[N_{u}A_{ul} + \left(N_{u}\frac{q_{l}}{q_{u}}B_{lu} - N_{l}B_{lu} \right) I_{\nu} \right]$$

The gain coefficient (g_v) is defined by¹¹

$$g_{\nu} = h\nu N_{A}\phi(\nu)B_{1u}\left(\frac{q_{1}}{q_{u}}N_{u} - N_{1}\right)$$
(B.5)

Thus,

$$\frac{\mathrm{dI}_{\nu}}{\mathrm{dx}} = \mathrm{h}\nu \,\mathrm{N}_{\mathrm{A}}\phi(\nu)\,\mathrm{N}_{\mathrm{u}}\mathrm{A}_{\mathrm{ul}} + g_{\nu}\mathrm{I}_{\nu}$$

Under lasing conditions, spontaneous emission has negligible effect on the intensity; the following approximation may then be made

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$$\frac{\mathrm{dI}_{\nu}}{\mathrm{dx}} = g_{\nu} I_{\nu} \tag{B.6}$$

This expression, however, only describes the change in intensity as the radiation passes through the active medium. In a laser cavity, there are additional factors that affect the intensity, notably the losses at the mirrors that form the cavity. Consider a cavity with homogeneous active medium of length (L) and enclosed by mirrors of reflectivity R_0 and R_L . The intensity, after one round trip in the cavity, is

$$I_{\nu}^{f} = I_{\nu}^{i} e^{2g_{\nu}I} R_{O}R_{L}$$
 (B.7)

The threshold condition is defined as that at which the intensity within the cavity neither increases nor decreases and the associated value of g_{ν} is the threshold gain ($\alpha_{\rm thr}$). Thus, at threshold

$$e^{2\alpha}$$
thr^L R_oR_L = 1 (B.8.a)

or

$$\alpha_{\text{thr}} = -\frac{1}{2L} \ln(R_0 R_L) \qquad (B.8.b)$$

Combining Equations (B.7) and (B.8), the change in intensity after one round trip in the cavity is

$$\Delta I_{\nu} = I_{\nu}^{f} - I_{\nu}^{i}$$
$$= I_{\nu}^{i} \left[e^{2g_{\nu}L} R_{o}R_{L} - 1 \right]$$
$$= I_{\nu}^{i} \left[e^{2L(g_{\nu} - \alpha_{thr})} - 1 \right]$$

For small departures from threshold,

$$e^{2L}(g_{\nu} - \alpha_{thr}) \cong 1 + 2L(g_{\nu} - \alpha_{thr})$$

Then,

$$\frac{\mathrm{dI}_{\nu}}{\mathrm{dx}} \cong \frac{\Delta \mathrm{I}_{\nu}}{2\mathrm{L}} \cong (g_{\nu} - \alpha_{\mathrm{thr}}) \mathrm{I}_{\nu}$$
(B.9)

For computational purposes, a photon flux (f_v) , in mol-cm⁻²-sec⁻¹, is defined as

$$f_{\nu} = \frac{I_{\nu}}{h\nu N_{A}}$$
(B.10)

The corresponding rate equation for this flux is

$$\frac{\mathrm{d}f_{\nu}}{\mathrm{d}x} = \frac{1}{c} \frac{\mathrm{d}f_{\nu}}{\mathrm{d}t} = (g_{\nu} - \alpha_{\mathrm{thr}})f_{\nu} \qquad (B.11)$$

Although Equation B. 11 was derived with the assumption that $L(g_v - \alpha_{thr})$ is small, the same result may be obtained by averaging the intensity, gain, and loss over the cavity.

DERIVATION OF X rad

APPENDIX C

APPENDIX C DERIVATION^{*} OF X_{rad}

The rate equation for $N_{HF(v,J)}$ is

$$\frac{dN_{HF(v,J)}}{dt} = X_{i} + X_{rad}(v,J) - X_{rad}(v-1, J+1) + A(v,J)$$
(C.1)

where X_i is the net change in $N_{HF(v,J)}$ resulting from chemical reactions and X_{rad} represents the change that results from stimulated emission and absorption

$$X_{rad}^{\nu} = X_{abs}^{\nu} + X_{st em}^{\nu}$$
(C.2)

the absorption term is⁶⁶

$$X_{abs}^{\nu} = -N_{1}B_{1u} \int \phi(\nu') I_{\nu} d\nu'$$

= -N_{1}B_{1u} \phi(\nu) I_{\nu} (C.3)

where the frequency integration is over the narrow laser bandwidth assumed to be at line center ν . The emission is

$$X_{st em}^{\nu} = N_{u}B_{ul} \int \phi(\nu') I_{\nu} d\nu'$$
$$= N_{u}B_{ul} \phi(\nu) I_{\nu} \qquad (C.4)$$

^{*}The derivation of Reference 11 is partially followed.

with Equations (B. 4), (C. 2), (C. 3) and (C. 4) combined

$$X_{rad}^{\nu} = \phi(\nu)B_{lu}\left(\frac{q_l}{q_u}N_u - N_l\right)I_{\nu}$$

and substituting from Equations (B.5) and (B.10),

$$X_{rad}^{\nu} = \frac{g_{\nu}I_{\nu}}{h\nu N_{A}}$$
$$= g_{\nu}f_{\nu} \qquad (C.5)$$

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are obtained.

DERIVATION OF THE ENERGY EQUATION

APPENDIX D

APPENDIX D

DERIVATION OF THE ENERGY EQUATION

The first law of thermodynamics is

$$dQ = dU + p dV$$

Applying the definition for enthalpy, h, this equation may be written as

$$dh = dQ + V dp \qquad (D.1)$$

Make the identifications

$$\frac{h}{V} = \sum_{i} N_{i}H_{i} \qquad (D.2.a)$$

$$\left(\frac{1}{v}\right)\left(\frac{dQ}{dt}\right) = -P_{L}$$
 (D.2.b)

where N_i is the molar concentration of species i, H_i is the molar enthalpy of species i, and P_L is the output lasing power per unit volume. Equation (D. 1) then becomes

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i} \mathrm{N}_{i} \mathrm{H}_{i} = -\mathrm{P}_{\mathrm{L}} + \frac{\mathrm{d}p}{\mathrm{d}t}$$

or

$$\sum_{i} N_{i} \frac{dH_{i}}{dt} + \sum_{i} H_{i} \frac{dN_{i}}{dt} = -P_{L} + \frac{dp}{dt}$$

For an ideal gas,

$$\frac{dH_{i}}{dt} = \left(\frac{dH_{i}}{dT}\right) \left(\frac{dT}{dt}\right) = C_{p_{i}}\left(\frac{dT}{dt}\right)$$
(D.3)

where C_{p_i} is the molar specific heat of species i at constant pressure. The energy equation then can be written

$$\sum_{i} N_{i} C_{p_{i}} \frac{dT}{dt} - \frac{dp}{dt} = -P_{L} - \sum_{i} H_{i} \frac{dN_{i}}{dt}$$
(D.4)

For computational purposes, an alternate form of this equation that does not contain explicitly the pressure variable is sought. For an ideal gas,

$$p = \sum_{i} N_{i}RT \qquad (D.5.a)$$

$$C_{p_i} - C_{v_i} = R$$
 (D.5.b)

By the differentiation of Equation (D.5.a) and the assumption that the density remains constant,

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \sum_{i} N_{i} R \left(\frac{\mathrm{d}T}{\mathrm{d}t}\right)$$

is obtained. The substitution of Equation (D.5.b) then leads to

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}\mathbf{t}} = \sum_{\mathbf{i}} N_{\mathbf{i}} \left(C_{\mathbf{p}_{\mathbf{i}}} - C_{\mathbf{v}_{\mathbf{i}}} \right) \left(\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}\mathbf{t}} \right)$$
(D.6)

The desired form of the energy equation is obtained by combining Equations (D.4) and (D.6); thus,

$$\sum_{i} N_{i} C_{V_{i}} \frac{dT}{dt} = -P_{L} - \sum_{i} H_{i} \frac{dN_{i}}{dt}$$
(D.7)

CALCULATION OF PULSE ENERGY

APPENDIX E

APPENDIX E

CALCULATION OF PULSE ENERGY

For the optical cavity shown in Figure E.1 (with the attenuator momentarily ignored),

$$I_{out} = (1 - R_0)I^{-1}$$
 (E.1.a)

$$I_{out}^{+} = (1 - R_L)I^{+}$$
 (E.1.b)

$$I = I^{-} + I^{+}$$
 (E.1.c)

and, from Reference 22,

$$\frac{I_{out}^{-}}{I_{out}^{-} + I_{out}^{+}} = \frac{1 - R_{o}}{\left[1 + (R_{o}/R_{L})^{1/2}\right] \left[1 - (R_{o}R_{L})^{1/2}\right]} \quad (E.1.d)$$

where I^- and I^+ are radiation intensities within the cavity in the negative and positive-x directions, respectively, I is the average intensity inside the cavity, and I^-_{out} and I^+_{out} are radiation intensities passing through mirrors R_o and R_L , respectively. (I^-_{out} is the predicted laser output from the model.)

With the attenuator in the position shown, the radiation lost from the cavity in the negative direction consists of three parts

$$I_{out}^{-} = I(1 - t) + I(1 - R_{o}) + I R_{o}(1 - t)$$
 (E.2)



Figure E.1. Optical cavity.

where t is the transmissivity of the attenuator. The three terms on the right-hand side of Equation (E.2) represent, respectively, the radiation reflected from the attenuator while traveling in the negative direction, the radiation passing through R_0 , and the radiation reflected from the attenuator after reflection from R_0 . The second term is the only portion actually seen by the detector and is the laser output. Equation (E.2) may be expanded and rewritten as

$$I_{out}^{-} = I^{-} \left(1 - t^{2} R_{o} \right)$$
 (E.3)

If

$$R'_{o} = t^2 R_{o}$$
 (E.4)

is defined, then

$$\mathbf{I}_{out}^{-} = \mathbf{I}^{-} (\mathbf{1} - \mathbf{R}_{o}') \tag{E.5}$$

With R'_{o} as the reflectivity of the output coupling, the model can be used to compute I_{out}^- . The actual output (I_L^-) , however, is given by

$$\frac{I_{L}}{I_{out}} = \frac{I[t(1 - R_{o})]}{I[(1 - t^{2}R_{o})]} = \frac{t(1 - R_{o})}{1 - t^{2}R_{o}}$$
(E.6)

DESCRIPTION OF COMPUTER SIMULATIONS FOR THE PULSED HF CHEMICAL LASER

APPENDIX F

APPENDIX F

DESCRIPTION OF COMPUTER SIMULATIONS FOR THE PULSED HF CHEMICAL LASER

Simulation of the pulsed HF laser is accomplished through two distinct computer models. The two systems modeled are: (1) the $H_2 + F_2$ chain reaction laser, where the rotational level populations are assumed to follow a Boltzmann distribution at the translational temperature, and (2) the SF₆-H₂ laser pumped by the F + H₂ reaction, where the individual rotational-level populations are determined from the solution of rate equations.

The basic structure of both models is similar. Each consists of a controlling main program, designated by MODEL, and four subroutines, designated GAIN, DIFSUB, DIFFUN, and FLASH. MODEL initiates the computational variables such as concentration, photon flux, temperature, and time; defines the cavity conditions; obtains reaction rate constants and necessary spectroscopic and thermodynamic data from data files; and provides the program control parameters that direct the program flow as well as the integration process. In the case of the SF₆-H₂ laser, MODEL also computes the rotational-relaxation rate constants, and provides the product energy distribution for the pumping reaction. Subroutine GAIN is used to compute the medium gain of the laser for any given

84
allowed P-branch transition by means of Equation (2.7). When this gain is found to be near or above the threshold value, the corresponding photon flux is monitored by MODEL for possible laser action.

Time progression within the model proceeds along the integration steps. Numerical integration is accomplished through the subroutine DIFSUB, which utilizes a modified Adams-Moulten technique developed by Gear.³⁵ Derivatives required for the integration are computed from rate Equations (2.2), (2.5), and (2.14) and obtained by means of the subroutine DIFFUN. Laser initiation by electrical discharge (or flash photolysis) may be modeled through the subroutine FLASH, which provides a timedependent F-atom production rate, based on the input power profile.

A flow chart describing the computer programs is presented in Figure F.1. This figure is an overview that displays the chain of commands and decisions that are followed to obtain ultimately the integrated values of the species concentrations within the laser medium as well as the photon flux density and temperature as a function of time.

The variables and symbols used in Figure F.1 and in the computer programs are defined in Tables F.1 and F.2. Bookkeeping limitations and computational practicability demand that the large number of time-dependent variables be grouped in an array. In addition, since the dimension of an array is changable, this provides the model with the flexibility of altering the number of variables under consideration. The array is two dimensional and is designated Y(I, J), J = 1, ..., N, where Y(1, J) represent the variables in question, N is the total number of such variables and Y(I, J), I > 1,



Figure F. 1. Computer simulation of pulsed HF chemical laser.

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are related to the (I-1)th derivatives of Y(1,J). Tables F. 1.a and F. 1.b define these variables as used in the $H_2 - F_2$ and the $SF_6 - H_2$ models, respectively. The other symbols found in the computer programs are defined in Table F.2.

Typical computer outputs from the model calculations at a selected time in the duration of the laser pulse are given in Tables F. 3 and F. 4. Table F. 3 is from the $H_2 + F_2$ model and Table F. 4 is from the SF_6-H_2 model. Complete listings of the programs and subroutines are given in Tables F. 5 through F. 12. Table F.1.a. Identification of variables Y(1,N) in $H_2 + F_2$ model

Y(1, N) Ν HF(v) concentration, mol-cm⁻³, v = N - 11-9 Undefined, reserved for additional variables 10-16 H-atom concentration, mol-cm⁻³ 17 $H_2(v)$ concentration, mol-cm⁻³, v = N - 1818-20 F-atom concentration, mol-cm⁻³ 21 F_2 concentration, mol-cm⁻³ 22 Translational temperature, °K 23 Photon flux, f(v, J), $mol-cm^{-2}-sec^{-1}$, v = |(N - 17)/7|, $J = J_{max}^{v} - 4$, \cdots , $J_{max}^{v} + 2$, where J_{max} indicates the transition of maximum gain. 24-79

Table F.1.b. Identification of variables Y(1, N) in SF_6-H_2 model

| 1 -7 | HF(v) concentration, mol-cm ⁻³ , $v = N - 1$ |
|--------|---|
| 8-23 | HF(0, J) concentration, mol-cm ⁻³ , J = 0, \cdots , 15 |
| 24-39 | $HF(1, J)$ concentration, mol-cm ⁻³ , $J = 0, \dots, 15$ |
| 40-55 | HF(2, J) concentration, mol-cm ⁻³ , J = 0, \cdots , 15 |
| 56-71 | HF(3, J) concentration, mol-cm ⁻³ , J = 0, \cdots , 15 |
| 72 | H-atom concentration, mol-cm ⁻³ |
| 73-75 | $H_2(v)$ concentration, mol-cm ⁻³ , v = N - 73 |
| 76 | F-atom concentration, mol-cm ⁻³ |
| 77 | F_2 concentration, mol-cm ⁻³ |
| 78 | Translational Temperature, °K |
| 79-125 | Photon flux f(v, J); specific values of v and J selected by the |

program

Ν

Table F.2. Nomenclature

| Symbol in Text | Symbol in Computer Program | Definition |
|---------------------------------|-------------------------------|--|
| A(v, J) | A(V,J) | Einstein isotropic coefficient for spontaneous emission, 1/molecule-sec |
| B(v, J) | B(V, J) | Einstein isotropic intensity absorption coefficient, cm ² /molecule-J-sec |
| с | С | Speed of light, 2.997925×10^{10} cm/sec |
| C _{Vi} | CVI | Molar specific heat at constant volume of species i, cal/mol-°K |
| E_{J}^{v} | E(V,J) | Rotational energy of state V, J, cm ⁻¹ |
| | F(T,J) | Resonance broadening function, Reference 22 |
| f(v, J) | FLUX(V,J) | Photon flux, mol-cm ⁻² -sec ⁻¹ |
| g(v, J) | ALPHA(V,J) | Gain of transition $(v + 1, J - 1) \rightarrow (v, J),$ cm ⁻¹ |
| h | | Plank's constant, 6.6256×10^{-34} J-sec |
| h | | Specific enthalpy, kcal/g |
| H _i | EHPYI | Molar enthalpy of species i, kcal/mol |
| I | CRRNT | Discharge current, amp |
| k | K | Boltzmann's constant, 1.38054×10^{-23} J-°K-1 |
| ^k r, ^k -r | KFR, KBR | Forward and backward rate constants, in terms of moles, centimeters, and sec- onds |
| L | LNTH | Length of active medium, cm |
| N _i | Y(1,I) | Concentration of species i, $mol-cm^{-3}$ |
| $\frac{dN_i}{dt}$ | DERVIY(I) | Time-derivative of N _i , mol-cm ⁻³ -sec ⁻¹ |

| Table F.2. | (Continued) |
|------------|--------------|
|------------|--------------|

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| Symbol in Text | Symbol in Computer Program | Definition |
|----------------------------------|-------------------------------|--|
| N _A | NA | Avogadro's number, 6.02252×10^{23} molecules-mol ⁻¹ |
| PL | POWER | Power density of laser output, $W-cm^{-3}$ |
| P _I | PIN | Power input from initiation, $W-cm^{-3}$ |
| Q_r^v | Q(V, T) | Rotational partition function for level v |
| ^R O ^R L | RO, RL | Mirror reflectivities |
| R | R | Universal gas constant, 1.98725 cal- mol ⁻¹ -°K-1 |
| t | Т | Time, sec |
| Т | Y(1,23) | Temperature, °K |
| α _{ri} ,β _{ri} | | Stoichiometric coefficients of reaction r |
| ^α thr | THGAIN | Threshold gain, cm ⁻¹ |
| φ(v,J) | PHI(V,J) | Normalized line profile of transition $(v + 1, J - 1) \rightarrow (v, J)$, cm |
| ۳ _R | TAU(V,J) | Rotational relaxation time constant, sec |
| ^ω c ^(v,J) | WC(V, J) | Wave number of transition $(v + 1, J - 1) \rightarrow (v, J), cm^{-1}$ |

Table F.3. Sample computer output for the $H_2 + F_2$ model.

SIEP SIZE= . 31252E-J7 SEC **DIFSUB CALLED 4529 TIMES**. PULSE ENERGY= .47045E-02 JOULES/CC TEMPERATURE= .50459E+03 K. LASING POWER= .62237E+02 WATTS/CC TIME= .76017E-04 SEC.

CONCENTRATIONS IN MOLES/CC

| | E-10 | | 72 | | | | | | | |
|---------------------|----------------------|------------------|---|--|----------------|--------------|---|---|-------------|--------------------------|
| | HF(8 .24998 | | MAX+3) 136-13 06-13 06-13 | | 06-13 06-13 | | 15-12 26-12 65-12 | 2E-12 | 26-12 | 5E-12 8E-12 |
| | F(7) 786E-16 | | F (V.) • 1000 • 1000 | | . 1000 | | • 42 88 • 4 3 1 1 | 1996 1996 1996 1997 1997 | .3671 | .3541 |
| | 0 . 57 | | •JMAX+2) 0006-13 0006-13 0006-13 | 00000-113 | 0106-13 | | 641E-12 815c-12 8245-12 | 525E-12 6025-12 | 300E-12 | 410E-12 431E-12 |
| 6 | HF (6) . 33651E-1 | | | | | | M | | 37 | |
| 333086-0° | 60- | | V • JMAX+11 0000E-13 8530E+00 | 9952E+00 0268E-13 3721E-03 | 00001-13 | | 43936-12 71486+02 | 23276+02 | 1711E-01 | 7405E+00 |
| . 80 | нғ (5) . 16691£ | | | | , . , . | | | | | ~~~ |
| H2(1) .22763E- | .35246E-09 | | F (V UMAX 10000E-1 10000E-1 10000E-1 | 10000000000000000000000000000000000000 | • 1000E - 1 | | . 45132E-1 . 45183E-1 | +1774E-1 | 51222E+0 | • 37043E-1 |
| H2(0) .242196-07 | .85935E-09 | SQUARED | F (V.JMAX-1) • 1 00006 - 1 3 • 1 00006 - 1 3 • 1 00006 - 1 3 | .10000E-13 | .10006-13 | | .45860E-12 .45846E-12 .43846E-12 | -423795-12 -403795-12 | .38987E-12 | •34081c-12 |
| .27312E-17 | .23272E-08 | IN MJLES/SEC/CH- | F(V,JMAX-2) 10000E-13 10000E-13 | | .16000E-13 | IN WATTS/CC | • 46575E-12 • 46496E-12 • 44445E-12 | • + 2 96 9E - 12 | . 39521E-12 | .38056E-12 .34604E-12 |
| .59477E-09 | .73901 6-0 8 | LASING LINES. | F (V, JMAX-3) • 10000E-13 • 10000E-13 | | .1000E-13 | TRANSITIONS. | .472795-12 .471305-12 | . + 3 5 4 4 - 1 2 . 4 3 5 4 4 - 1 2 . 4 4 4 4 4 - 1 2 | .400396-12 | .38539E-12 .35114E-12 |
| 6 20E- 08 | (0) 49E-07 | LUX OF THE | лах 12 94 | ማወኲ | ٥٥ | THE LASING | 7 1 9 | n ao at | | ወጥ |
| .14 | . 363 | PHOTON F | >040 | เพรเก | 0 | POWER OF | 540 | um-1 | . م | 91 |

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CONTRIBUTION TO PULSE ENERGY FROM EACH TRANSITION IN JOULES/CC

| 00000000000000000000000000000000000000 | | 84444444488888888888888888888888888888 |
|--|-------------------|--|
| 00000000000000000000000000000000000000 | | 94444 690000000000000000000 69440000000000000000 694400000000000000 6044000000000000 6040000000000 |
| 400000 400000 400000 40000 40000 40000 40000 40000 400000 | | 54440000000000000000000000000000000000 |
| L 3400 200 200 L 300 200 L 300 200 L 300 200 L 300 200 L 310 | | |
| 00000000000000000000000000000000000000 | | t 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 |
| 40000000000000000000000000000000000000 | IN 1/CM | -100111110 -100111110 -100010000000 -10000000000 |
| HE (1) 304 8.5(-1.2) 3394 8.5(-1.2) 3394 8.5(-1.2) -33394 8.5(-1.2) -33394 8.5(-1.0) -2222 776-05 -2222 776-05 -2522 776-05 -2527 77 | IBLE TRANSITIONS, | AL PHA(1, 1) AL |
| 8477666664 8777664 8777664 87776464 87777647 87777647 87777777777 | AIN FOR ALL POSS | the state of |
| ๅ๚൜ฅ ๕฿๏๛๏฿๏๚๗ฅํ๚ ๚๚๚๚๚ | THE G | - วศุญษายุณฑายุ อศุภษายุ |

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| model. |
|-------------------|
| 6 ^{-H} 2 |
| SF |
| output for |
| Computer |
| Sample |
| F.4. |
| Table |

| = 3HI 1 | .1063JE-06 SEC | TEMESI | RATLRE= .418 | 49E+03 K, | DIFSU3 CALLED | 1360 TIMES, | STEP SIZE= .27103 | 3E-10 SEC |
|-------------------------------|---|-------------------|--------------|---------------------|----------------------|---------------------|-----------------------|--------------|
| ASIN | 6 PONE9= 46917 | E+05 WATTS/CC | PUL S | 5E ENEFGY= .75407 | E-D3 JOULES/CC | | | |
| CONCE | NTRATICNS IN 401 | LES/CC | | | | | | |
| - | .33679£-C7 | .4166.5-27 | С. F2 | +2(0) .10354E-C5 | н2(1) .51396Е-39 | H2(2) .20624E-12 | | |
| มะคงคะเจอง400tmmen C คลคลค | K - 400 - 40 - 30 - 40 - 40 - 40 - 40 - 4 | | | | HF (4) .24821E-10 | .56571E-13 | нғ(б) . 31343Е-16 | |
| | POWER OF LASIN | 5 LINES (HDTTS/C(| 0 | ENERGY CF EACH L | INE (JOULES/CC) | GAIN OF | EACH POSSIBLE TRANSIT | ION (1/CM) |
| ٦ | ΗF (0, J) | HF(1,J) | HF(2,J) | HF (C, J) | FF(1,J) HF | (2,J) ALPFA(| C,J) ALPHA(1,J) 4 | AL PHA (2,J) |

| AL PHA (2,J) | 0000 + 00000000 |
|---------------|--|
| AL PHA (1,J) | 10 30 41 41 40 40 40 40 40 40 40 40 40 40 40 40 40 |
| ALP+A (C , J) | 0000000 1 000000 |
| HF(2,J) | 50 |
| FF(1,J) | 500 501 11 502 502 502 502 502 502 502 502 |
| HF(0,J) | |
| HF(2,J) | 7.1 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0 |
| HF(1,J) | 05000 0000000 |
| ΗF(0,J) | 000000 00000000 ••••• ••• ••• ••• ••• •• |
| ٦ | ๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛๛ |

ROTATIONAL RELAXATION TIME (SEC)

HF(3, U)

FF(2,J)

Table F.5. Program MODELC

*DECK MODELC PP) GRAM MODELC(INPUT, OUTPHT, TAPE1, TAPE2, TAPE3, TAPE4, TAPE7, TAPE8, TAPES, TAPE10, TAPE11, TAPE12) 1 DITENSION V(8,79), DERVIV(79), STORE(7) CO1MON YMAX(79), SAVF(12,79), ERROR(79), PH(6400), E(10,31), HC(9,18), B(9,14),0(9,61),F(50,30),KFR(142),KBR(142),ALPHA(8,15), 1 JMAX(3), CVF(17), CVF2(17), EHPYH(17), EHPYH2(17), EHPYF(17), 1 EHPYE? (17), EHOVHE (17), THGAIN, PL, FLUX, CVN2 (17), AR, HE, N2, 1 RCTF(142), PGTR(142), PF(142), SIGNL(8), PLINE(8, 15), ELINE(8, 15) 1 REAL KER, KBP , N2 PE10(1,60)E REVD(2,10) WG RFND(3,10)8 REID(4,10)0 REVD(10,10)F PFID(8,50)CVF, CVF2, CVN2, CVSF6, CVH2, CVHF RFID(9,20)FHOYH, FHPYH2, FHPYF, EHPYF2, EHPYHF 10 FORMAT(5E16.5) 20 FOR MAT (5F16.5,/5F16.5/5F16.5/2F16.5,48X) 30 FOLMAT(E20.8) 50 FOLMAT(5F16.5) 60 FORMAT(5F14.5) RH? = 1. RF! = . 98 R=1 = . 94 PH: = 50. PN? = 0. PA2 = 0.KE1 = 23 FCTR = .5142E-7------FLJX=1.F-14 TI4EL = 200.E-6DF.MIN = 1.F-15ALLM = DELMIN/100. H = .4 F-10 HMIN = DELMIN HM1 X = 2.F-7 $EP_{3} = 1 \cdot F - 1$ MACDER = A R0 = 0.8 RL = 1. LNFH = 100.TSCIP = 1.E-6 TS'EP = TSKIP NOT = 7 JCIT=25 JGVIN = JONT POTER = 0.EN; Y = 0.PL = 1. T = 0. JSTAPT = 0MF = 0 00.990 I = 1,8 $J_{M} X (I) = 4$ 30 990 J = 1,15 PL[NF(I, J) = 7.EL[NF(I, J) = n.

```
Table F.5. (Continued)
  990 AL'HA(I,J) = 0.
      DO 1000 I = 1,125
 1000 Y = 1.E-6
      00 1005 I=1,142
      RC^{\dagger}F(I) = 0.
      PC(B(I) = 0.
 1005 RF(I) = 0.
      HE = RHE + FOTR
      Nº = RN2 + FCTR
      \Delta \mathbf{R} = \mathbf{P} \Delta \mathbf{P} + \mathbf{F} \mathbf{C} \mathbf{T} \mathbf{P}
      T+;AIN = -ALOG(RO + PL)/(2. + LNTH)
      DO 1010 I = 1, 17
1010 Y(L, I) = 0.
      Y(L,18) = PH2 + FOTO
      Y(1, 19) = 0.
      Y(1,20) = 0.
      Y(1, 21) = PE1 + ECTE
      Y(1,22) = PF2 + FCT=
      Y(L,23) = 300.
      DO 1020 I = 24,79
1020 \forall (l, I) = FLUX
      AK^{2} = (Y(1,23) - 10^{0})/25 + 1.5
      KT: IFIX(AKT)
      00 1022 T=1,KT
      REVD(12,30) KF9
 1022 REID(7,30) KAP
 1025 TO. 7 = T
      AI(T = (Y(1, 23) - 100.)/25. + 1.5
      IK' = IFIX(AIKT)
1030 IF(KT.EQ.IKT) GO TO 1050
KT) IF = TKT - KT
      IF(KTDIF.GT.0) GO TO 1035
      PRINT 1033
1033 FOLMAT (// TEMPERATUPE HAS DROPED#//)
      60 TO 1190
 1035 \text{ KT} = \text{IKT}
      07 1040 I = 1,KTDIF
   ----
      REVD(12,30) KFR
1040 RFID(7,30) K8P
1050 IF(T.E0.0.) GO TO 1139
      J31IN = JGATN + 1
      IF(JGAIN - JCNT) 1054,1058,1058
<u>C</u>
C..........COMPUTE GAIN FOF THE LINES NEAR J-MAX
C
1054 DO 1056 I=1,8
      IV: I-1
      JL)W = JMAX(\underline{T}) - \overline{T}
      J_{IGH} = J_{MAX}(I) + 3
-----
      30 1056 J=JLOW, JHIGH
 1056 ALPHA(T,J) = GAINC(IV, J, 79, Y)
G0 TO 1130
C .... JO CHECK FOR J-SHIFT
C
1058 \text{ JGVIN} = 0
   00\ 1060\ I = 1,8
      IV = I - 1
      D0 \ 1060 \ J = 1,15
1060 \text{ ALPHA(I,J)} = \text{GAING(TV,J,79,Y)}
```

```
Table F.5. (Continued)
C,
                             (LOWER LEVEL) OF MAX GAIN
C.....DETERMINE THE J
<u>.</u>____
      00 1120 I = 1,8
      JMXXO = JMXX(I)
      JHX(I) = 4
      JM = 4
      00 \ 1070 \ J = 5.13
      IF(ALPHA(I,J).LF.ALPHA(I,JM)) GO TO 1070
.. ....
      JMIX(I) = J
      J^{\mu} = J^{\mu} \Lambda X(I)
 1070 CONTINUE
      IF( JMAX(I) . EQ. 4) 50 TO 1075
-----
      JM(X(I) = JMAX(I) - 1
 1075 CONTINUE
      IF(JMAX(I).EQ.JMAXO) 50 TC 1123
C
C.....IF A J-SHIFT HAS OCCUPRED, REDEFINE THE APPROPRIATE F(V,J) AND
С
      JSLAPT = 0
      LJ = JMAX(I) - JMAXO
      L = 7 * I + 15
      IF(LJ.LT.0) GO TO 1192
      IF(LJ.GE.7) GO TO 1101
      K^{c} = 7 - LJ
      DO 1080 M = 1,KS
1080 Y(L,L+M) = Y(1,L+LJ+M)
      D0 1090 N = 1, LJ
 1090 Y(L, L+N+KS) = FLUX
      GO TO 1120
 1197 \text{ NL} = -LJ
      IF[NLJ.GE.7) GO TO 1100
      NKS = 7 - NLJ
DO 1193 M=1, NKS
----
 1193 \text{ ST} = Y(1, L+M)
      20 1194 M=1, NKS
1194 Y(L, L+NLJ+M) = STOPF(M)
      D0 1195 M=1, NLJ
1195 Y(L,L+M) = FLUX
      Gn TO 1120
 1100 DO 1110 M = 1,7
1110 Y(L,L+M) = FLUX
 1120 CONTINUE
C
C......INTEGRATE
С
 1130 CA.L DIFSUB(79,T,Y, SAVE, H, HMIN, HMAX, EPS, MF, YMAX, ERFOR, KFLAG,
                   JSTAPT, MAXDEE, PW, KEY)
     1
      NCT = NCT + 1
      GO TO 1136
 1134 H = HMTN
      HM[N = HMIN/2C.
      JS^{r}ART = -1
      50 TO 1139
1136 CONTINUE
      IF: KFLAG.LE. 0) GO TO 1150
      D0 1610 I=24,79
      IF(Y(1,I).LT.FLUX) Y(1,I)=FLUX
```

```
Table F.5. (Continued)
1610 CONTINUE
      H1 = T - TOLD
      COIST=2.85912 + THGAIN
      POVER =0.
      DO 1137 T=1.8
      K=1MAX(I) - 4
      L=" #I+16
      00 1137 J=1,7
      PL[NF(I,K+J) = Y(1,L+J) + WC(I,K+J) + CONST + 4.184
      POIER = POWEP + PLINE(I,K+J)
1137 ELINE(I,K+J) = FLINE(I,K+J) + PLINE(I,K+J) + H1
      ENLY = ENGY + POWEP + +1
      IF(T.GT.TIMEL) 60 TO 1139
      IF(T.LE.TSTER) 50 TO 1149
      TSLEP = TSTEP + TSKTP
1139 PR: NT 1140.T, Y(1, 23), NCT. H1
1140 FORMAT(#1TIME=*,E11.5,* SFC,*,10X,*TEMPERATURE=*,E11.5,* K,*,
     1 1) X, *DIFSUR CALLFO*, 16, * TIMES, *, 10X, *STEP SIZE=*, F11.5, * SEC*)
      PPINT 1410, POWER, FNGY
1410 FORMAT(/* LASING PONEP=*,E11.5,* WATTS/00*,10X,* PULSE ENERGY=*,
             F11.5,* JOULFS/CC*)
     1
      PP[ NT 1510
1510 FORMAT(///* CONCENTRATIONS IN MOLES/CC*)
      PO[ NT 1141
1141 FORMAT(/ 11X, +H+, 15Y, +F+, 14X, +F2+, 12X, +H2(0)+, 12X, +H2(1)+, 12X,
                #H2(2)#)
     1
      P°[NT 1142, Y(1, 17), Y(1, 21), Y(1, 22), Y(1, 18), Y(1, 19), Y(1, 20)
1142 FOLMAT(6F16.5)
      PRENT 1143
1143 FORMAT(//7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*,10X,
                *HF(4)*,10X,*HF(5)*,10X,*HF(6)*,10X,*HF(7)*,10X,*HF(8)*)
     1
     PRINT 1144, (Y(1, I) \cdot I = 1, 9)
1144 FOR MAT(9E15.5)
      PP[NT 1520
1528 FORMAT(///# PHOTON FLUX OF THE LASING LINES, IN MOLFS/SEC/CM-SQUAR
    1E71)
      PR[NT 1145
1145 FOR MAT(/ 4X, +V+, 9X, +JMAX+, 4X, +=(V, JMAX-3) +, 5X, +F(V, JMAX-2) +, 5X,
             *F(V, JMAX-1) *.5X, *F(V, JMAX)*, 5X, *F(V, JMAX+1)*, 5X,
     1
             *F(V, JMAX+2) *, 5X, *F(V, JMAX+3) *)
     1
      DO 1147 I = 1,9
      IV = I - 1
      L : 7 * I + 15
      \tilde{P}^{\circ}: NT 1146, IV, JMAX(I), (Y(1,L+J), J = 1,7)
1146 FORMAT(15,110,7F16.5)
1147 CONTINUE
      PRENT 1530
1530 FORMAT(///* POWER OF THE LASING TRANSITIONS, IN WATTS/CC*/)
      DO 1540 I=1,8
      IV: I-1
      K=JMAX(I) - 4
      PC[NT_1146, IV, JMAY(I), (PLINE(I, K+J), J=1, 7)
 1540 CONTINUE
      PR[ NT 1550
 1550 FORMATE * 100NTPIBUTION TO PULSE ENERGY FROM FACH TRANSITION IN JOUL
     1ES/ CC+)
      PP[ NT 1560
 1560 FOZ MAT(/3X,+J+,RX,+HF(0,J)+,9X,+HF(1,J)+,9X,+HF(2,J)+,9X,+HF(3,J)+
     1.9(.+HF(4.J) +.9X.+HF(5.J) +.9X.+HF(6.J) +.9X.+HF(7.J) +)
      DO 1570 J=1.15
      PP: NT 1210, J, (FLINE (I, J), I=1, 8)
```

·

```
1579 CONTINUE
      PP[ NT 1589
 1580 FORMAT(///* THE SAIN FOR ALL POSSIBLE TRANSITIONS, IN 1/CM+)
      PP[ NT 1200
 1200 FORMAT (//34, +J+,64, +ALPHA(0, J) +,64, +4LPHA(1, J) +,64, +4LPHA(2, J) +,
             5X, # ALPHA (3, J) #, 6Y, # ALPHA (4, J) #, 6X, # ALPHA (5, J) #, 6X, # ALPHA (6
     1
     1, J #, 6X, #ALPHA (7, J) *)
      00 1220 J=1,15
      PP[NT 1210, J, (ALPHA(T, J), I=1,8)
1210 FORMAT(14,8516.5)
1220 CONTINUE
      IF(T.EO. 0.) GO TO 1130
      IF(T.GT.159.F-6.AND. POWEF.LT.1.E-1) GO TO 1170
1149 JSTART = 1
1310 IF(T.LF.TIMEL) 60 TO 1025
      GO TO 1170
1150 IF(HMIN .GE. ALTM) GO TO 1134
      PPENT 1160, KFLAG, T
1160 FOR MAT(1X, *STEP UNSUCCESSFUL*//15, E16.5)
      CALL DIFFUN(T,Y, DFPV1Y)
      PRENT 1165, DFPV1Y
1165 FOR MAT (/1X, 5E16.5)
      GO TO 1190
1170 PRENT 1180
1180 FORMAT(1X, #UPPER LIMIT OF INTEGR ATION REACHED#)
1190 CONTINUE
      EN)
```

Table F.6. Subroutine GAINC

```
*DECK GAL NC
      FUICTION GAING(IV.J.N.Y)
C
      THES FUNCTION CALCULATES THE GAIN OF A P-BRANCH TRANSITION WITH
r,
C
      LOIER LEVEL HE (V. J)
      THES SUBPOUTINE TO DE USED WITH PROGRAM MODELC.
C,
С
      DITENSION Y(8,79)
      CO4MON YMAX(79),SAVF(12,79),ERROR(79),PW(6400),E(10,31),WC(9,18),
            B(9,18),Q(9,61),F(50,30),KFR(142),KBR(142),ALPHA(8,15).
     1
             JMAX(3), CVF(17), CVF2(17), EHPYH(17), EHPYH2(17), EHPYF(17),
     1
             EHPYF2(17), EHPYHF(17), THGAIN, PL, FLUX, CVN2(17), AR, HE, N2,
     1
             ROTF(147), POTP(147), FF(147), SIGNL(8), PLINE(8,15), FLINE(8,15)
     1
      RELL NUP. NON .N2.LONTZ
      TE4 = Y(1,23)
      AIF = TEM/100. + .5
      IT = IFIX(AIT)
      A1 = 0.0705230784
      A2 = 0.0422820123
      A3 = 0.0092705272
      A4 = 0.0001520143
      A5 = 0.0002765672
----
      A6 = 0.0000430638
      WHF = 20.01
      DO>P = 3.5811338E-7 #WC(IV+1,J) # SORT(TEM/WHF)
      WT11=0.
      WT12=0.
      00 10 I=1,6
      WT41=WTM1 + Y(1,I)
   10 \text{ HT}_{12} = \text{HT}_{12} + Y(1, 1+16)
      WT42 = WTM2 + HE + M2 + AP
      WT4 = 1.74 * (WTM1 + Y(1.7) + Y(1.8) + Y(1.9)) + .865 * WTM2
      LOATZ = A2.057 + SOPT(TFM) + (WTM + Y(1, IV + 1) + F(IT, J) + ((
               252./SOPT(TEM)) - 1.74))
     1
YL:NE = 0.83255461 + LONT7 / D)PP
      IF( YLINE.GT. (?.4)) GO TO 20
     PHE = (0.46971864/DOPP) * EXP(YLINE*YLINE)
      PHL = PHI = (1. + A1 = YLINE + A2 = YLINE**2 + A3 = YLINE**3 + A4
-----
     1* /LINF**4 + 45 * VLINE**5 + 46 * YLINE**6)**(-16)
     GO TO 30
20 COIST = 2. * YLINE**2
      PH[ = (1. - CONST + (-1) + 3. + CONST + (-2) - 15. + CONST + (-3)]
     1+ L05. * CONST**(-4))/(3.1415926535 * LONTZ)
<u>30 NU<sup>3</sup> = (Y(1, IV+2) + (2. + FLOAT(J) -1.)/Q(IV+2, IT+1)) + EXP(-1.4387856</u>
            *E(IV+2,J)/TEM)
     1
     ND4 = (Y(1, IV+1)* (2. * FLOAT(J)+1.)/Q(IV+1, IT+1))*EXP(-1.4387886
            #F(IV+1, J+1)/*EM)
   .... 1 ..
     GA[NC = 3.1753646F-11 * WC(IV+1,J) * PHI * B(IV+1,J) * (((2. *
              FLOAT(J) +1.)/(2. + FLOAT(J) - 1.)) + NUP - NDN)
    1
PELUKN
     EN)
```

Table F.7. Subroutine DIFFUNC

*JECK DIFFUNG SUBROUTINE DIFFUN(T,Y,DEFV1Y) c C THIS SUBROUTINE TO BE USED WITH MODELC <u>C</u>_ DIIENSION Y(8,79), DEPV1Y(79), VVHF(8), VTHF(8), VTH2(8), SEM(8) COINON YMAX(79), SAVF(12,79), ERROP(73), PW(6400), E(10,31), WC(9,18), 1 B(9,14),Q(9,61),F(F0,30),KFR(142),K3R(142),ALPHA(8,15), JMAX(8), CVF(17), CVF2(17), EHPYH(17), EHPYH2(17), EHPYF(17), 1 EHPYF2(17), EHPYHF(17), THGAIN, PL, FLUX, CVN2(17), AP, HE, N2, 1 RCTF(147), RCTF(147), RF(142), SIGNL(8), PLINE(8,15), FLINE(3,15) 1 RELL 41, M2, M3, M4, M5, M6, M7, M8, M3, M10, KEP, KBP, N2 M5 = Y(1,1)D1 10 I = 2,9 10 M5 = M5 + Y(1,I)M4 = Y(1, 17)M9 = Y(1,18) + Y(1,19) + Y(1,23)FSJM = Y(1, 21) + Y(1, 22)HEVRE = HE + AR + ESUM M1 = M5 + 2.4 + FSUM + HE + AR + M9 + M4 M2 = M5 + HEAPE + 2.5 * M9 + 20. * 44 + N2 MR = M5 + HEARE + M9 + M4 + N2 M6 = Y(1, 21)M7 = Y(1,22) + ARN9 = HE 41) = HEARE + 4. # 49 + 4. # M4 + N2 C THE FOLLOWING ARE THE COLD PUMPING REACTIONS C С DO 20 I = 1,6 RCFF(10+I) = Y(1,18) * Y(1,21) * KFR(10+I) 20 RC(B(10+I) = Y(1,17) * Y(1,1+I) * KBP(10+I) C C THE FOLLOWING ARE THE HOT PUMPING REACTIONS C $D0 \ 30 \ I = 1,9$ RC(F(16+I) = Y(1,17) * Y(1,22) * KFR(16+I) 30 RC[B(16+I) = V(1,21) * V(1,I) * KBR(16+I) C THE FOLLOWING APE THE V-T DEACTIVATION REACTIONS C C 00 40 I = 1,8- -RC[F(25+1) = 45 + Y(1,1+1) + KFR(25+1) RC[8(25+T) = N5 + Y(1,I) + KBR(25+I) RC[F(33+I) = M5 + Y(1,I+1) + KFP(33+I) RC[B(33+1) = M5 + Y(1,1) + KBR(33+1) RC[F(41+I) = M6 + Y(1,I+1) + KER(41+I)RC(B(41+T) = M6 + Y(1,I) + KBR(41+I) RC[F(49+I) = 47 + Y(1,I+1) + KFR(49 + I)RC[B(49+I) = 47 + Y(1,I) + KBR(49+I)RCFF(93+1) = M8 * Y(1,1+1) * KFR(93+1) - - - - -FC[9(97+1) = M8 + Y(1,1) + KBP(93+1)PC(F(101+I) = M9 * Y(1,I+1) * KFR(101+I) RC[9(101+I) = M9 * Y(1,I) * KBR(101+I) <u>c</u> C THE FOLLOWING ARE MULTI-QUANTA V-T DEACTIVATIONS <u>C</u> RC[F(57+1) = M4 + Y(1,9) + KFR(57+1) 49 PC[9(57+1) = M4 + Y(1,9-1) + K33(57+1) 00 50 I = 1.7

```
RC[F(65+1) = 44 + Y(1,8) + KFR(65+1)]
   50 RC(B(65+I) = M4 + Y(1,8-I) + K3R(65+I)
      00.60 I = 1,6
      RC[F(72+1) = 44 + Y(1,7) + KFP(72+1)
   60 RC(B(72+I) = M4 + Y(1,7-I) + K3R(72+I)
      00.70 I = 1,5
      RC[F(78+1) = M4 + Y(1.6) + KFR(78+1)
    70 RC(B(78+I) = M4 + Y(1,6-I) + K9R(78+I)
      00 80 I = 1,4
      RC[F(83+1) = H4 + Y(1,5) + KFR(83+1)
   80 RC(B(A3+I) = M4 + Y(1,5-I) + K3R(A3+I)
      90 I = 1,3
      RC(F(87+1) = M4 * Y(1,4) * KFR(87+1)
   90 \text{ RC}^{\circ} B(87+I) = M4 + Y(1,4-J) + K3R(87+I)
      DO 100 I = 1,^{2}
      RC[F(90+I) = M4 + Y(1,3) + KFR(90+I)
  100 RC*B(90+I) = M4 * Y(1,3-I) * K37(90+I)
      RC[F(93) = 44 + Y(1,2) + KFF(93)
      PC*B(93) = M4 + Y(1.1)+KPF(93)
S
C THE FOLLOWINE ARE HE-HE V-V EYCHANGE REACTIONS (NEGLECT 117, 124, 13)
C
      DO 119 I= 1,7
      RC^*F(109+I) = Y(1,I+1) + Y(1,I+1) + KFR(109+I)
  110 RC[B(109+I) = Y(1,I) * Y(1,I+2) * K3R(109+I)
      D0 120 I = 1,6
      RCFF(117+I) = Y(1,I+1) + Y(1,I+2) + KFR(117+I)
  120 RGFB(117+I) = Y(1,I) * Y(1,I+3) * K3R(117+I)
      DO 130 I=1,5
      PC'F(124+I) = Y(1,I+1) * Y(1,I+3) * KFR(124+I)
  130 RC[B(124+T) = Y(1,T) + Y(1,T+4) + K^{2}R(124+T)
      00 140 I=1.4
      RC(F(130+I) = Y(1,I+1) * Y(1,I+4) * KFR(130+I)
 RC'B(130 +I) = Y(1, T) * Y(1, I+5) * (BR(130+I)
C
C THE FOLLOWING ARE HE-HE V-V EXCHANGE REACTIONS
C
      RC[F(134+I) = Y(1,I) + Y(1,19) + KFR(134+I)
  140 RC'B(134+I) = Y(1,I+1) * Y(1,18) * KBR(134+I)
      DO 150 I=1,?
      PC'F(138+T) = Y(1,I) * Y(1,20) * KFR(138+I)
      R(138+I) = Y(1,I+1) + Y(1,19) + KBR(138+I)
C
  THE EDLOWING ARE V-T DEAGTIVATIONS FOR H2(V)
C.
C
       RCFF(140+I) = 410 * Y(1,18+I) * KFR(140 +I)
  150 RC(3(140+1) = M10 * Y(1,17+1) * KBR(140 +1)
       30 \ 160 \ I = 11,142
  169 RF(I) = PCTF(I) - RCTB(J)
1
C VTHE(I) IS THE V-T DEACTIVATION RATE OF HE FROM HE(I) TO HE(I-1)
С
     DO 165 I=1,8
  165 VT4F(I) = RF(25+I) + PF(33+I) + RF(41+I) + RF(49+I) + RF(93+I) +
                 RF(101+I)
С
  VTH2(I I IS THE V-T DEACTIVATION RATE OF H2 FROM H2(I) TO H2(I-1)
С
С
VT12(1) = RF(135) + RF(136) + RF(137) + RF(138) + RF(141)
```

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```
VT12(2) = RF(139) + RF(140) + RF(142)
C
  THE PUIPING TERMS SUMMED
C
C
      CD_{1}D_{2} = PF(11) + RF(12) + PF(13) + RF(14) + RF(15) + RF(16)
      HOT =_RF(17) + RF(1A) + RF(19) + RF(20) + RF(21) + PF(22) + RF(23)
            + PF(24) + RF(25)
C VVMF(I) APE SOME V-V EXCHANGE TERMS FOR HE-HE. ADD TO HE(I-1) TERM
2
      VV1F(1) = RF(118) + RF(125) + RF(131) - RF(135) - PF(139)
      VVIF(2) = RF(119) + RF(126) + PF(132) - RF(136) - PF(140)
      VV(F(3) = -RF(118) + PF(120) + RF(127) + RF(133) - PF(137)
      VVIF(4) = -PF(119) + RF(171) - RF(175) + RF(128) + RF(134) - RF(138)
      VVIF(6) = -RF(121) + PF(123) - PF(127) - RF(132)
      VV(F(5) = -RF(120) + PF(122) - RF(126) + RF(129) - PF(131)
      VVIF(7) = -FF(122) - PF(128) - RF(133)
     VVIF(A) = -PF(123) - PF(129) - RF(134)
C
C TIME PERIVATIVE OF THE CONCENTRATIONS DUE TO CHEMISTRY CNLY
<u>,</u>
      DE(VIY(1) = PF(17) + RF(65) + RF(72) + RF(78) + RF(83) + FF(87) +
                  RF(90) + FF(92) + RF(93) + RF(110) + VTHF(1) + VVHF(1)
     1
      DF&V1Y(2) = PF(11) + PF(18) + &F(64) + RF(71) + RF(77) + RF(82) +
                  PF(86) + PF(89) + PF(91) - RF(93) - 2. * RF(110) +
     1
                   PF(111) - VTHF(1) + VTHF(2) - VVHF(1) + VVHF(2)
     1
      DF&V1Y(3) = RF(12) + RF(19) + RF(63) + RF(70) + RF(76) + RF(81) +
                  RF(85) + PF(88) - RF(91) - RF(92) + RF(110) -
     1
                  2. * RF(111) + RF(112) - VTHF(2) + VTHF(3) - VVHF(2) +
     1
                   VVHF(3)
     1
      DFLV1V(4) = PF(13) + PF(20) + RF(62) + PF(69) + PF(75) + PF(80) +
                  PF(84) - RF(88) - RF(89) -RF(90) + RF(111) -
     1
                   2. * RF(112) + RF(113) + VTHF(4) - VTHF(3) + VVHF(4) -
     1
                  VVHF(3)
     1
      DF2V1Y(5) = RF(14) + RF(21) + RF(61) + RF(58) + RF(74) + PF(79) -
                  RF(84) - RF(85) - RF(86) - RF(87) + RF(112) -
     1
.....
                  2. * RF(113) + RF(114) + VTHF(5) - VTHF(4) + VVHF(5) -
    1
                  VVHF(4)
     DELV1Y(6) = RF(15) + PF(22) + PF(60) + PF(67) + RF(73) - RF(73) -
                  FF(80) - RF(81) - RF(82) - RF(83) + RF(113)
    1
                  - ?. # FF(114) + RF(115) + VTHF(6) - VTHF(5) + VVHF(6)
    1
                  - VVHF(5)
     DF&V1Y(7) = FF(16) + RF(23) + RF(59) + RF(56) - RF(73) - RF(74) -
----
                  FF(75) - PF(76) - RF(77) - RF(78) + RF(114) -
    1
                  2. * RF(115) + RF(116) + VTHF(7) - VTHF(6) + VVHF(7) -
    1
                  VVHF(6)
     1
     DF&V1Y(8) = RF(24) + RF(58) - RF(66) - RF(67) - RF(68) - RF(69) -
                  RF(70) - RF(71) - RF(72) + RF(115) - 2. * RF(116) +
    1
                  VTHF(R) = VTHF(7) + VVHF(R) = VVHF(7)
     1
     DF(V1V(9) = PF(25) - PF(58) - RF(59) - RF(50) - RF(51) - RF(62) -
                  RF(53) - RF(64) - RF(65) + RF(116) - VTHF(8) - VVHF(8)
     1
     DO 170 T = 10,16
 170 DELVIY(I) = 0.
      DERVIY(17) = COLD - HOT
      DF(V1Y(18) = VTH2(1) - CCLO
     DF(V1Y(19) = VTH(2) - VTH(2)
      DESVIV(20) = -VTH2(2)
      DE(V1Y(21) = -DERV1Y(17))
```

```
DEVIY(22) = -HOT
C
C EFFECT OF RADIATION ON HE(V) CONCENTRATION
C
      SI;NL(I) IS TOTAL PATE OF EMISSION FROM HE(I) TO HE(I-1)
C
      DO 190 T = 1,8
      L = 7 + T + 16
      K = JMAX(T) - 4
  180 ST; NL(I) = ALPHA(I,K+1) + Y(1,L+1) + ALPHA(I,K+2) + Y(1,L+2) +
                  ALPHA(1, K+3) + Y(1, L+3) + ALPHA(1, K+4) + Y(1, L+4) +
     1
                  ALPHA(I,K+5) * Y(1,L+5) + ALPHA(I,K+6) * Y(1,L+6) +
     1
                  ALPHA(I, K+7) * Y(1, L+7)
     1
      DF(V1Y(1) = DFRV1Y(1) + SJGNL(1)
      DFRVIY(9) = DFPVIY(9) - SIGNL(8)
      DO 190 I = 2,8
  190 \text{ DERVIY(I)} = \text{DERVIY(I)} + \text{SIGNL(I)} - \text{SIGNL(I-1)}
C
 CALCULNTE OUTPUT POWER
Č
С
С
      HC'AVAGADRO NO. = 2.85912 CAL-CH/HOLE
      COIST = 2.85912 # THGAIM
      PL = 0.
      DO 200 I = 1,8
      K = JMAX(I) - 4
      L = 7 + I +16
      D) 200 J = 1,7
  208 PL = PL + Y(1,L+J) + WC(T,K+J)
      PL = PL + CONST
C
C TEMPERITURE DERIVATIVE
<u>C</u>
      AII = Y(1,23)/100. + .5
      IT = IFIX(AIT)
      CVSUM = 2.981 * (HE + AR + Y(1,17)) + CVN2(IT) * N2 +
              5.076 + (Y(1,18) + Y(1,19) + Y(1,20)) + 5.020 + (Y(1,1) +
     1
              Y(1,2) + Y(1,3) + Y(1,4) + Y(1,5) + Y(1,6) + Y(1,7) +
     1
              Y(1,8) + Y(1,9)) + CVF(IT) * Y(1,21) + CVF2(IT) * Y(1,22)
     1
      ETILPY = ((EHPYH(IT) + 52.102) - (EHPYF(IT) + 18.900)) *DERV1Y(17)
                +(EHPYF2(IT)) * DERV1Y(22) + (EHPYH2(IT)) * DERV1Y(18)
     1
                +(EHPYH2(IT) + 11.889) # DERV1Y(19)
     1
                +(EHPYH2(IT) + 23.112) * DERV1Y(20)
     1
     1
                +(EHPYHF(IT) - 64.800) + DERV1Y(1)
                +(EHPYHF(IT) - 53.473) + DERV1Y(2)
     1+(:HPYHF(IT) - 42.638) * () CRV1Y(3) + (EHPYHF(IT) - 32.282) *
     1DE&V1Y(4) + (EHPYHF(IT) - 22.392) + DERV1Y(5) + (EHPYHF(IT) -
     1 12.959) * DERVIY(6) + (EHPYHF(IT) - 3.973) * DERV1Y(7) +
     1 (:HPYHF(IT) + 4.572) * DERVIY(3)+(EHPYHF(IT)+12.680)*DERVIY(9)
      ETILPY = ETHLPY + 1.E+3
      DF(V1Y(23) = -(PL + ETHLFY) / GVSUM
   -
      00 210 T = 1,8
      L = 7 + I + 16
      K = JMAX(I) - 4
      CO 210 J = 1,7
  210 DF(V1Y(L+J) = (ALPHA(I,K+J)-THGAIN) * 2.997925E+10 * Y(1,L+J)
      30\ 220\ I = 24,79
  220 IF(Y(1,I) .LE .FLUX . AND .DERVIY(I) .LT.0.) DERVIY(I) = 0.
      RETURN
      EN)
```

Table F.8. Program MODELG

PROGRAM MONFLS(INPUT, JUTPUT, TAPE1, TAPE2, TAPE3, TAPE4, TAPE7, TAPE8, TAPE9, TAPE10, TAPE11, TAPE12, TAPE13) 1 C.....MORELS USES THE SAME RATES AND MATRIX ELFMENTS AS MODELC DIMENSION Y(8,125), DERVIY(125), XXX(34), YMAX(125), SAVE(15,125), ERR) . P(125), PW(15000) COMMON E(10,31), ELVL(3),CVF(17),CVF2(17),EHPYH(17),FHPYH2(17),EHPYF(17), 1 EHPYF2(17), EHPYHF(17), THGAIN, PL, FLUX, CVN2(17), AR, HE, N2, 1 PCTF(142), PCTB(142), RF(142), SIGNL(4), PLINE(3,15), WC(9,18), 1 ELINF(3,15), TAU(4,16), BOLTZ(4,16), HFVJ(4,16), SF6, 1 CVSF6(17), CVH2(17), CVHF(17), FLUXJ(3, 15), MFLAG(3, 15), 1 NFLAG(3,15), NVAR, NPVAR, FPRODA, SLOP(3,19), TRCEP(3,19) PFAL KFR, KPP, N2 PEAD(1,69) F READ(2,10) WC PEAD(3,10)8 READ(4,10) 0 READ(10,10)F READ(8,50) CVF, CVF2, CVN2, CVSF6, CVH2, CVHF READ(9,20) FHPYH, EHPYH2, EHPYF, EHPYF2, EHPYHF READ(11,40) SLOP, TRCEP 10 FORMAT(5E16.5) 20 FORMAT(5F16.5/5F16.5/5F16.5/2F16.5,48X) 30 FORMAT(520.8) 40 FOPMAT(F15.5) 50 FORMAT(5F16.5) 60 FORMAT (5E14.5) C ----- PARTIAL PRESSURES (TORR) RF?=0. FF1=0. ---------. RH2=4. RHE =40. $\frac{RN2}{RAR} = 0.$ KEY =78 RSF6=4. FCTR=.5348F-7 FLUX=1.E-14 $TIMEL = 1 \cdot E - 6$ H1=0. $DELMIN = 1 \cdot E - 15$ ALTM = DELMIN/100. H = .4 E-10 HMIN = DELMIN $HMAX = 2 \cdot F - 7$ FPS=1.F-1 MAXOFR = 8 RL = .5 R0=.95 LNTH=169. TSKIP=5.F-9 TIMEL=3.0F-6 TSKIP=.1F-6 TSTEP = TSKIP NRVAR = 78 NVAR = NPVAR NCT = 0 KKK=0

```
POWER = 0.
       ENGY = 0.
       PL = 1.
       T = 0.
       JSTART = 0
       MF = 0
       10990 I = 1,3
       FLVL(I) = 0.
       00 990 J = 1,15
       FLUXJ(I,J) = FLUX
       MFLAG(I,J) = 0
       NFLAG(I,J) = 0
       PLINF(I,J) = 0.
       ELINE(I,J) = 0.
   990 ALPHA(I, J) = 0.
       DO 1000 T = 1,125
  1000 MAX(I) = 1.E-6
       00 1005 I=1,14?
       RCTF(1) = 0.
      PCTB(I) = 0.
 1005 RF(I) = 0.
      HE = PHE + FOTR
       N2 = RN2 + FCTP
       AP = RAP + FOTR
       SES = PSES + FOTR
       THEAIN = -ALOG(PO + RL)/(2. + LNTH)
      00 1010 T=1,125
1010 Y(1,T) = 0.
       Y(1,73) = PH2 + FCTR
       Y(1,74) = 0.
  Y(1,75) = 0.
       Y(1,76) = PF1* FCTR
       Y(1,77) = RF2 + FCTR
       Y(1,78) = 300.
       AKT = (Y(1,78) - 100.)/25. + 1.5
       KT=IFIX(AKT)
 DO 1022 I=1,KT
       PEAD(12, 30) KFR
  1022 READ(7,30) KBR
       ITDROP=0
  1025 TOLD = T
       AIKT = (Y(1, 78) - 100.)/25. + 1.5
       IKT = IFIX(AIKT)
  1030 IF(KT.EQ.IKT) GO TO 1050
       KTOIF = IKT - KT
       IF(KTDIF.GT.0) GO TO 1035
       PPINT 1033, Y(1,78)
  1033 FORMAT(//* TEMPERATURE HAS DROPPED NEW TEMPERATURE IS*,F10.5//)
ITOROP=ITOPOP+1
       GO TO 1050
  1035 \text{ KT} = \text{IKT}
00 1040 I = 1,KTDIF
       READ(12,30) KFP
  1040 PEAD(7,30) KAR
1050 ABT = Y(1,78)/100. + 1.5
       IBT=IFIX(ABT)
       00 1051 I=1,4
       00 1051 J=1,16
```

```
BOLT7(I,J)=((2.*FLOAT(J)-1.)/Q(I,IBT))*EXP(-1.4387886*
                   E(I,J)/Y(1,78))
      1
 1051 HFVJ(I, J) = Y(1, I) * BOLTZ(I, J)
                                         . . .
       TAUA=2.E-8/Y(1.78) **.5
       XI=1.E-3
       \begin{array}{r} D0 & 1054 \ \text{I}=1,4 \\ D0 & 1054 \ \text{J} = 1,16 \end{array}
----
                                             - ----
  1054 TAU(I,J)= TAUA* EXP(1.4387886*XI*(E(I,J+1)-E(I,J))/Y(1,78))
       IF(T.ED. 0.) SO TO 1139
                                                     LFLAG=0
 C....SINGLE LINE ON P(2,3)
    ALPHA(2,3)=GAING(1,3,125,Y)
       DO 1100 I=1,3
       IV = I - 1
       00 1100 J=1,15
 C
                                            ) Y, 521, J, VI (GNIAG = ) J, I(AH^{2})
 C.....CHECK FOR LINES NEAR OR ABOVE THRESHOLD
  <u>IF(ALPHA(I,J) - .1 + THGAIN) 1060,1080,1080</u>
1060 IF(FLUXJ(I,J) - 1.E-5) 1070,1080,1080
  1070 NFLAG(I,J) = 0
FLUXJ(I,J) = FLUX
       PLINE(I,J) = 0.
       GO TO 1090
 1080 \text{ NFLAG}(I, J) = 1
  1090 IF(NFLAG(I,J) .FQ. MFLAG(I,J)) GO TO 1100
       LFLAG = LFLAG + 1
  1100 CONTINUE
 C.....TF THE SET CF VARIABLES HAS NOT CHANGED, PROCEED TO INTEGRATION
 C..... IF THE SET HAS CHANGED, DEFINE NEW VARIABLES AND REINITIALIZE.
IF(LFLAG .LE. 0) GO TO 1130
                                                                .....
       JSTART = 0
       NVAR=NPVAR
       DO 1110 I=1,3
 00 1110 J=1,15
       IF(NFLAG(I, J) .LE. 0) 50 TO 1110
NVAP = NVAR + 1
       Y(1, NVAR) = FLUXJ(I, J)
                                                             ----
  1110 CONTINUE
 <u>C</u>
 C....INTEGRATE
 С
  1130 CALL DIFSUB(NVAP, T, Y, SAVE, H, HMIN, HMAX, EPS, MF, YMAX, ERROR, KFLAG,
JSTART, MAXDER, PW, KEY)
      1
       NCT = NCT + 1
       GO TO 1136
  1134 H = HMIN
       HMIN = HMIN/20.
       JSTART = -1
      GO TO 1130
  1136 CONTINUE
       IF(KFLAG.LE. N) GO TO 1150
DO 1610 I=79,NVAR
       IF(Y(1,1).LT.FLUX) Y(1,1)=FLUX
                                                           1610 CONTINUE
      H1 = T - TOLD
----
      CONST=2.85912 + THGAIN
      POWER =0.
 MVAR = NRVAR
```

| 00 1120 I=1,3 |
|---|
| FLVL(I) = 0. |
| <u>50 1120 J=1,15</u> |
| MFLAG(I,J) = NFLAG(I,J) |
| IF(NFLAG(I,J) .LE. 0) GO TO 1120 |
| |
| FLUXJ(I,J) = Y(I,HVAR) |
| PLINE(I,J) = FLUXJ(I,J) + WC(I,J) + CONST + 4.184 |
| POWER = POWER + PLINE(1,J) |
| ELINE(I,J) = FLINE(I,J) + PLINE(I,J) + HI |
| ELVL(I) = ELVL(I) + ELINE(I,J) |
| |
| FNGT = FNGT + FUNER + 11 |
| $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |
| |
| 14 TO OPTAT 11/A.T.Y(1.7A) ANT.H1 |
| 11/9 FORMAT(#1TIME=+,F11,5,# SEC.#.10%,#TEMPERATURE=#,F11,5,# K.#. |
| 1 104-4DTESUB CALLED* 16-4 TIMES * 104-4STEP STZE * 11.5.* SEC4) |
| OPTNT 1441. DOMER. ENGY |
| 1410 FORMATINE HASHING POWER=+,F11,5,+ WATTS/CC+,10%,+ PULSE ENERGY=+, |
| 1 F11-5-* JOULES/CC*) |
| |
| 1510 FORMAT(//# CONCENTRATIONS IN MOLES/CC#) |
| PRINT 1141 |
| 1141 FORMAT(/ 11X.*H*.15X.*F*.14X.*F2*.12X.*H2(0)*.12X.*H2(1)*.12X. |
| 1 + H2 (2) *) |
| PPINT 1142. Y (1.72) . Y (1.76) . Y (1.77) . Y (1.73) . Y (1.74) . Y (1.75) |
| 1142 FORMAT(6F16.5) |
| |
| PRINI LIGO |
| 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, |
| 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) |
| 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) |
| <pre>PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7)</pre> |
| <pre>PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,I),I=1,7)</pre> |
| <pre>PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5)</pre> |
| <pre>PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 00X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16</pre> |
| PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) NC 2010 K=1,16 J=K-1 |
| <pre>PKINT 114.5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) NC 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K)</pre> |
| <pre>PRINT 114.5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) NC 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5)</pre> |
| <pre>PRINT 114.5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 114-5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 1145 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 114-5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 114-5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 114-5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 114.5 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1</pre> |
| <pre>PRINT 1143 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 00X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,]),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PPINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(///7X,*POWER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EA3 1H LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(7,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPHA(1,J)*,4X,*ALPHA(2,J)*/)</pre> |
| 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PPINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FORMAT(15,4E15.5) 2010 CONTINUE PRINT 1570 1520 FORMAT(///7X,*POWER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EAC 14 LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(/3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 #HF(0,J)*,7X,*HF(1,J)*,7X,*ALPHA(0,J)*,4X, 1 ALPHA(1,J)*,4X,*ALPHA(2,J)*/) 00 1540 J=1,15 |
| <pre>PRINT 1143 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 00X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PPINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(///7X,*POWER OF LASING LINES (HATTS/CC)*,10X,*ENERGY OF EA3 1H LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(9,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPHA(1,J)*,6X,*ALPHA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3),</pre> |
| <pre>1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5)</pre> |
| <pre>1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,I),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+4),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(//7X,*POWER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EAD 1H LINE (JOULES/CC)*,11X,*GAIN DF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(/3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPHA(1,J)*,4X,*ALPHA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), 1540 CONTINUE</pre> |
| <pre>1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,I),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2910 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(//7X,*POHER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EAC IH LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/GH)*) PRINT 1530 1530 FORMAT(/3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(9,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPHA(1,J)*,4X,*ALPHA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), 1 (ALPHA(I,J),I=1,3) 1540 CONTINUE 1550 FORMAT(I4,9F14.5) </pre> |
| <pre>PRINT 1143 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 00X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+4),Y(1,39+K),Y(1,55+K) 1144 FORMAT(15,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(///7X,*POHER OF LASING LINES (HATTS/CC)*,10X,*ENERGY OF EA2 14 LINE (JOULFS/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(/3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, *ALPHA(1,J)*,4X,*ALPHA(2,J)*/ 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), (ALPHA(1,J),I=1,3) 1540 CONTINUE 1550 FORMAT(14,9F14.5) PRINT 3000</pre> |
| <pre>PRINT 1143 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 0C 2010 K=1,16 J=K-1 PPINT 1144,J,Y(1,7+K),Y(1,23+K),Y(1,39+K),Y(1,55+K) 1144 FOPMAT(15,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(///7X,*POHER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EA2 1H LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(0,J)*,7X,*HF(1,J)*,7X,*HF(1,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPMA(1,J)*,5X,*ALPHA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), 1 (ALPHA(1,J),I=1,3) 1540 CONTINUE 1550 FORMAT(14,9F14.5) PRINT 3000 3000 FORMAT(///* POTATIONAL RELAXATION TIMF(SEC)*)</pre> |
| <pre>PRINT 1143 1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+4),Y(1,39+K),Y(1,55+K) 1144 FORMAT(15,4E15.5) 2010 CONTINUE PRINT 1570 1520 FORMAT(///7X,*POHER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EA3 1H LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//3X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(9,J)*,7X,*HF(1,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPHA(0,J)*,4X, 1 *ALPHA(1,J)*,6X,*ALPHA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(1,J),I=1,3),(ELINE(I,J),I=1,3), (ALPHA(I,J),I=1,3) 1540 CONTINUE 1550 FORMAT(//* POTATIONAL RELAXATION TIMF(SEC)*) PRINT 3000 3000 FORMAT(//* POTATIONAL RELAXATION TIMF(SEC)*)</pre> |
| <pre>1143 FORMAT(//4X,*J*,7X,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,I),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+(),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(///7X,*POHER OF LASING LINES (HATTS/CC)*,10X,*ENERGY OF EAD 1H LINE (JOULFS/CC)*,11X,*GAIN DF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(/X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *ALPHA(1,J)*,4X,*ALPHA(2,J)*/ C0 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), (ALPHA(I,J)*,4X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X,*HF(3,J)* PRINT 3000 3000 FORMAT(///* POTATIONAL RELAXATION TIMF(SEC)*) PRINT (73X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X,*HF(3,J)* PRINT 7010 3010 FORMAT(//*,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X,*HF(3,J)*</pre> |
| <pre>1143 FORMAT(//X,*J*,*J*,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PRINT 1144,J,Y(1,7+K),Y(1,23+4),Y(1,39+K),Y(1,55+K) 1144 FORMAT(15,4E15.5) 2010 CONTINUE PRINT 1570 1520 FORMAT(///7X,*POHER OF LASING LINES (MATTS/CC)*,10X,*ENERGY OF EA2 1M LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//,7X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1</pre> |
| <pre>1143 FORMAT(//AX,*J*,*J*,*HF(0)*,10X,*HF(1)*, 10X,*HF(2)*,10X,*HF(3)*, 1 10X,*HF(4)*,10X,*HF(5)*,10X,*HF(6)*) PRINT 2001, (Y(1,1),I=1,7) 2001 FORMAT(5X,7E15.5) 00 2010 K=1,16 J=K-1 PPINT 1144,J,Y(1,7+K),Y(1,23+4),Y(1,39+K),Y(1,55+K) 1144 FORMAT(I5,4E15.5) 2010 CONTINUE PRINT 1520 1520 FORMAT(//7X,*POWER OF LASING LINES (WATTS/CC)*,10X,*ENERGY OF EA2 1H LINE (JOULES/CC)*,11X,*GAIN OF EACH POSSIBLE TRANSITION (1/CM)*) PRINT 1530 1530 FORMAT(//X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X, 1 *HF(7,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,5X,*ALPMA(0,J)*,4X, 1 *ALPMA(1,J)*,4X,*ALPMA(2,J)*/) 00 1540 J=1,15 PRINT 1550,J,(PLINE(I,J),I=1,3),(ELINE(I,J),I=1,3), 1540 CONTINUE 1550 FORMAT(///* POTATIONAL RELAXATION TIMF(SEC)*) PRINT 3010 3000 FORMAT(///* POTATIONAL RELAXATION TIMF(SEC)*) PRINT 7010 3010 FORMAT(/7X,*J*,6X,*HF(0,J)*,7X,*HF(1,J)*,7X,*HF(2,J)*,7X,*HF(3,J)* 1/) 00 3920 J=1,16</pre> |

```
PRINT 3030, JJ, (TAU(I, J), J=1, 4)
  3020 CONTINUE
  3030 FORMAT(14,4F14,5)
      KKK=KKK+1
      00 1730 J=1,15
XXX (J) = ALPHA (2, J)
      XXX(15+J)
                =PLINF(2,J)
  1230 CONTINUE
XXX (31)
               =Y(1,78)
      XXX (32)
               =POWEF
      XXX(33) = Y(1,76)
      XXX(34) = T
. . . . .
      WPITE(13,40) XXX
      PRINT 40,XXX
   IF(T.E0.0.) GO TC 1139
      TF(T.GT.1.E-6.AND.POWER.LT.5.E-3)30 TO 1170
  1149 JSTART = 1
1310 IF (T.LE. TIMEL) GO TO 1025
      GO TO 1170
  1150 IF(HMIN .GF. ALIM) GO TO 1134
                                        . . . . . .
                                                   ----
----
      PRINT 1160,KFLAG,T
1160 FORMAT(1X, *STEP UNSUCCESSFUL*//15, E16.5)
      CALL DIFFUN(T, Y, DERV1Y)
      PRINT 1165, DERVIY
1165 FORMAT(/1X,5E16.5)
                                                   GO TO 1190
  1170 PRINT 1180
1180 FORMAT(///1X, "UPPER LIMIT OF INTEGRATION PEACHED")
      PRINT 1185, KKK
  1185 FORMAT(//# KKK=#,15)
1190 CONTINUE
      IF(ITDPOP.GT.9) PPINT 1933, Y(1,79)
      FND
```

Table F.9. Subroutine GAING

```
FUNCTION GAING(IV, J.N.Y)
C
С
      THIS FUNCTION CALCULATES THE GAIN OF A P-BRANCH TRANSITION WITH
      LOWFP LEVEL HE(IV, J)
Ç
     THIS SUBROUTINE TO BE USED WITH PROGRAM MODELG.
С
С
      DIMENSION Y(9,125)
      COMMON F(10,31).
            P(9,18),0(9,61),F(50,30),KFR(142),KBR(142),ALPHA(3,15),
     1
            ELVL(3), CVF(17), CVF2(17), EHPYH(17), FHPYH2(17), EHPYF(17),
     1
            EHPYF2(17), EHPYHF(17), THGAIN, PL, FLUX, CVN2(17), AR, HE, N2,
     1
     1
            PCTF(142), PCTB(142), RF(142), SIGNL(4), PLINE(3, 15), WC(9,18),
            ELINF(3,15), TAU(4,16), BOLTZ(4,16), HFVJ(4,16), SF6,
     1
            CVSF6(17), CVH2(17), CVHF(17), FLUXJ(3,15), PFLAG(3,15),
     1
            NFLAG(3, 15), NVAR, NRVAR, FPPODA, SLOP(3, 19), TRCEP(3, 19)
     1
      PEAL NUP, NON. N2, LONTZ
      TEM = Y(1,78)
      AIT = TEM/100. + .5
      IT = IFIX(AIT)
      41 = 0.0705230784
      A_{2} = 0.0422829123
      A3 = 0.0092705272
      A4 = 0.0001520143
      A5 = 0.0002765672
      A6 = 0.0000430538
      WHE = 20.01
      DOPP = 3.5811338F-7 #WC(IV+1,J) # SQRT(TEM/WHF)
      WTM1=0.
      WT 42=0.
      DO 10 1=1,6
      WTM1=WTM1 + Y(1,I)
   10 WTM2 = WTM2 + Y(1, I+71)
      WT42 = WTM2 + 4F + N2 + AR + SF6
      WTM = 1.74 * (WTM1 + Y(1,7)) + .865 * WTM2
      LONT? = 82.057 * SQRT(TEH) * (WTM + Y(1,IV + 1) * F(IT,J) * ((
              257./SQPT(TEM)) - 1.74))
     1
      YLINE = 0.83255461 + LONTZ / DOPP
      IF(YLINE.GT.(2.4)) GO TO 20
      PHI = (0.45971864/00PP) + EXP(YLINE+YLINE)
      PHI = PHI * (1. + A1 * YLINE + A2 * YLINE**2 + A3 * YLINE**3 + A4
     1* YLTNE**4 + A5 * YLINE**5 + A6 * YLINE**6)**(-16)
      GO TO 30
   20 CONST = 2. + YLINE**2
      PHT = (1. - CONST + (-1) + 3. + CONST + (-2) - 15. + CONST + (-3)
     1+ 105. * CONST**(-4))/(3.1415926535 * LONT7)
   30 IMU=TV#16 + 23 + J
      IML = IV + 15 + 8 + J
      GAING = 3.1753646E-11 * WC(IV+1,J) * PHI * B(IV+1,J) * (((2. *
     1
               FLOAT(J) +1.)/(2. + FLOAT(J) - 1.)) + Y(1,IMU) - Y(1,IML))
      RETURN
      ENT
```

Table F.10. Subroutine DIFFUNG

```
SUBROUTINE DIFFUN(T, Y, DERV1Y)
 C
   THIS SUBPOUTINE TO BE USED WITH MODELS.
 C
 C
        DIMENSION Y(8,125), DERV1Y(125), VVHF(6), VTHF(6), VTH2(2)
        COMMON E(19,31),
              B(9,18),0(9,61),F(50,30),KFR(142),KRP(142),ALPHA(3,15),
       1
              FLVL (3), CVF (17), CVF2(17), EHPYH (17), FHPYH 2(17), EHPYF (17),
       1
              FHPY5?(17), EHPYHF(17), THGAIN, PL, FLUX, CVN2(17), AR, HE, N2,
       1
              RCTF (142), RCTB (142), RF (142), SIGNL (4), PLINE (3, 15), WC (9, 18),
       1
              ELINE(3,15), TAU(4,16), BOLTZ(4,16), HFVJ(4,16), SF6,
       1
              CVSF6(17), CVH2(17), CVHF(17), FLUXJ(3, 15), MFLAG(3, 15),
       1
              NFLAG(3,15), NVAR, NRVAR, FPRODA, SLOP(3,19), TRCEP(3,19)
     _ 1
        PEAL M1, M2, M3, M4, M5, M6, M7, M8, M9, M10, KFR, KBF, N2
       M5 = Y(1.1)
        00 1^{n} I = 2,7
    10 M5 = M5 + Y(1,I)
        M4 = Y(1,72)
        M9 = Y(1,77) + Y(1,74) + Y(1,75)
        FSUM = Y(1.76) + Y(1.77)
        HFARF = HE + AF + FSUM + SF6
        M1 = M5 + ?.4 * FSUM + HE + AR + M9 + M4 + SF6
          = M5 + HEARE + 2.5 # M9 + 20. # 44 + N2
        M2
        M3 = M5 + HEARF + M9 + M4 + N2
        M6 = Y(1,76)
                                        . . . . . . . . . .
        M7 = Y(1,77) + AR + SF6
        M8 = HE
        M10 = 4FARF + 4. * M9 + 4. * 44 + N2
 C
 C THE FOLLOWING ARE THE COLD PUMPING REACTIONS
C
                           ----
                                  ---
        00 20 I = 1,6
        RCTF(10+I) = Y(1,73) * Y(1,76) * KFR(10+I)
    20 RCTB(10+1) = Y(1,72) + Y(1,1+1) + KBR(10+1)
 С
 C THE FOLLOWING ARE THE V-T DEACTIVATION REACTIONS
 <u>Ç</u>__
                            . . . . .
        00 4^{1} I = 1,6
        RCTF(25+I) = 45 * Y(1,I+1) * KFR(25+I)
        PCTB(25+1) = M5 + Y(1,1) + KBR(25+1)
        RCTF(33+1) = M5 + Y(1,1+1) + KFR(33+1)
        RCTB(33+I) = M5 + Y(1,I) + KBR(33+I)
      RCTF(41+T) = 46 + Y(1, I+1) + KFR(41+T)
        RCTB(41+T) = M6 * Y(1,I) * KBR(41+I)
        RCTF(49+T) = 47 + Y(1,I+1) + KFR(49 + I)
        PCT8(49+1) = M7 * Y(1,1) * KBR(49+1)
        RCTF(93+1) = MR + Y(1,1+1) + KFR(93+1)
        RCTP(93+1) = M8 * Y(1,1) * KBR(93+1)
        RCTF(101+I) = 49 + Y(1,I+1) + KFR(101+I)
    40 RCTB(101+I) = M9 * Y(1, I) * K3R(101+I)
 С
   THE FOLLOWING ARE MULTI-DUANTA V-T DEACTIVATIONS
 С
 C
        0060I = 1,6
        RCTF(72+1) = M4 # Y(1,7) # KFR(72+1)
     60 \ \text{PCTB(72+T)} = M4 + Y(1,7-T) + KBR(72+T)
        00 \ 70 \ I = 1,5
        RCTF(78+1) = M4 * Y(1,6) * KFR(78+1)
     70 RCTB(74+1) = 44 + Y(1,6-1) + KBR(79+1)
```

```
DO \ 80 \ I = 1,4
      RCTF(83+1) = M4 # Y(1,5) # KFR(83+1)
   80 RCTB(83+T) = M4 + Y(1,5-I) + KBR(83+I)
      70 \ 90 \ I = 1, 3
      PCTF(87+1) = M4 * Y(1,4) * KFR(87+1)
   90 RCTR(87+J) = M4 + Y(1,4-J) + KBR(87+J)
      00 \ 100 \ I = 1,?
      RCTF(90+I) = M4 + Y(1,3) + KFR(90+I)
  100 RCTR(90+1) = M4 + Y(1,3-1) + KBR(90+1)
      RCTF(93) = 44 + Y(1,2) + KFR(93)
      PCTB(93) = M4 + Y(1,1) + KBR(93)
С
S THE FOLLOWINE APE HE-HE V-V EXCHANGE REACTIONS
C
      00 110 I= 1,5
   PC*F(109+I) = Y(1,I+1) * Y(1,I+1) * KFR(109+I)
  110 RCTB(109+I) = Y(1,I) * Y(1,I+2) * KBR(109+I)
      50 1?0 I = 1,4
 . . . . .
      PCTF(117+I) = Y(1,I+1) + Y(1,I+2) + KFR(117+I)
  120 RCTR(117+I) = Y(1,I) * Y(1,I+3) * KEF(117+I)
      00 1₹0 I=1,3
    - -
      RCTF(124+1) = Y(1,1+1) * Y(1,1+3) * KFR(124+1)
  130 RCTP(124+I) = Y(1,I) * Y(1,I+4) * KER(124+I)
   00 135 I=1.2
      RCTF(130+I) = Y(1,I+1) * Y(1,I+4) * KFR(130+I)
  135 RCTF(130 +I) = Y(1,I) + Y(1,I+5) + KBR(130+I)
C
          C THE FOLLOWING ARE HE-H2 V-V EXCHANGE REACTIONS
С
      00 140 I=1,4
      PCTF(134+I) = Y(1,I) + Y(1,74) + (FP(134+I))
  140 RCTP(134+I) = Y(1,I+1) * Y(1,73) * KBR(134+I)
      DO 150 I=1.2
      RCTF(138+I) = Y(1,I) + Y(1,75) + KFR(138+I)
      RCTP(138+I) = Y(1,I+1) + Y(1,74) + K9R(138+I)
C
C THE FOLLOWING APE V-T DEACTIVATIONS FOR H2(V)
С
      PCTF(140+I) = M10 * Y(1,73+I) * KFR(140 +I)
 150 RCTP(140+I) = M10 + Y(1,72+I) + K3R(140 +I)
      150 I = 11,142
  160 PF(I) = RC^{T}F(I) - RCT3(I)
С
C VTHE(I) IS THE V-T DEACTIVATION RATE OF HE FPOM HE(I) TO HE(I-1)
С
      00 165 I=1,6
  165 VTHF(I) = PF(25+I) + RF(33+I) + RF(41+I) + RF(49+I) + RF(93+I) +
                RF(101+I)
С
C VTH2(I) IS THE V-T DEAGTIVATION RATE OF H2 FROM H2(I) TO H2(I-1)
С
      VTH2(1) = #F(135) + RF(136) + RF(137) + RF(138) + RF(141)
      VTH2(2) = PF(139) + RF(140) + RF(142)
C
 THE PUMPING TEPMS SUMMED
С
С
     COLD = RF(11) + PF(12) + RF(13) + RF(14) + RF(15) + RF(16)
Ç_____
                                 . . .
```

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```
C VVHF(I) ARE SOME V-V EXCHANGE TERMS FOR HE-HE. ADD TO HE(I-1) TERM
С
      VVHF(1) = FF(118) + RF(125) + RF(131) - RF(135) - RF(139)
      VV4F(2) = PF(119) + RF(126) + RF(132) - RF(136) - RF(140)
      VVHF(3) = -RF(118) + RF(120) + RF(127) + RF(133) - RF(137)
      VVHF(4) = -PF(119) + RF(121) - RF(125) + RF(128) + RF(134)-RF(138)
      VVHF(6) = -RF(121) + RF(123) - RF(127) - RF(132)
      VVHE(5) = -PE(120) + 3E(122) - RE(126) + EE(129) - RE(131)
C,
C TIME DEPIVATIVE OF THE CONCENTRATIONS DUE TO CHEMISTRY ONLY
C
      DEPV1Y(1) = FF(17) + RF(65) + RF(72) + RF(78) + RF(83) + RF(87) +
                   RF(90) + RF(92) + RF(93) + RF(110) + VTHF(1) + VVHF(1)
     1
      DEPV1Y(2) =
                            RE(18) + RE(64) + RE(71) + PE(77) + RE(82) +
                  FF(86) + RF(89) + RF(91) - RF(93) - 2. * RF(110) +
     1
                  RE(111) - VTHE(1) + VTHE(2) - VVHE(1) + VVHE(2)
     1
      DERV1Y(3) =
                            RF(19) + RF(63) + RF(70) + RF(76) + RF(81) +
                  PF(85) + RF(88) - RF(91) - RF(92) + PF(110) -
     1
                   7. * RF(111) + RF(112) - VTHF(2) + VTHF(3) - VVHF(2) +
     1
                   VVHF(3)
     1
                            RF(20) + RF(62) + RF(69) + RF(75) + RF(80) +
      DERV1Y(4) =
                  PF(84) - RF(88) - RF(89) -RF(90) + PF(111) -
     1
                   ?. * RF(11?) + RF(113) + VTHF(4) - VTHF(3) + VVHF(4) -
     1
     1
                   VVHF (3)
      PEPV1Y(5) = PF(14) + RF(21) + RF(61) + PF(68) + RF(74) + RF(79) -
                  PF(84) - RF(85) - RF(86) - RF(87) + RF(112) -
     1
                   2. * RF(113) + RF(114) + VTHF(5) - VTHF(4) + VVHF(5) -
     1
                   VVHF(4)
     1
      DERV1Y(6) = RF(15) + RF(22) + RF(50) + RF(67) + RF(73) - RF(79) -
                   RF(A0) - RF(B1) - RF(B2) - RF(B3) + FF(113)
     1
   _ 1_
                   - ?. # RF(114) + RF(115) + VTHF(6) - VTHF(5) + VVHF(6)
                   - VVHF(5)
     1
      NFPV1Y(7) = PF(16) + RF(23) + RF(59) + RF(66) - RF(73) - RF(74) -
                  RF(75) - RF(76) - RF(77) - RF(78) + RF(114) -
     1
                  2. * RF(115) + RF(116) - VTHF(6) - VVHF(6)
     1
 ----- F DISSOCTATION = .05+SF6 FOR FPROD=4.E-2
C
      FPP004=.836E-3
      FPROD=FPRODA*FLASH(T) **2
C ----- FNFRGY IMPUT = 2.43JJULES/574 CC FOR PA=3.78F3
      PA=7.90F?
      DO 170 I=1,4
      CC 170 J=1,15
      IM=I#15+J-9
  170 DERV1Y(IM) = DEEV1Y(I) + ADLTZ(I,J) + (HEVJ(I,J) - Y(1,IM)) / TAJ(I,J)
      00 178 I=2.4
      KF=9+1
      K=1-1
      00 174 J=1,16
      IM = I + 16 + 1 - 9
  174 DERVIY(IM) = DERV1Y(IM) + (SLOP(K, J) *Y(1,78) +TRCEP(K, J))*RF(KF)
  178 DERVIY(I) = DERVIY(I) + RE(KE)
      9F9V1Y(72) = 00LP
      DERVIY(73) = VTH2(1) - COLD
      DFRV1Y(74) = VTH2(2) - VTH2(1)
      PERV1Y(75) = -VTH2(2)
      DER V1Y(76) =-DEE V1Y(72) +EPROD
```

```
Table F.10. (Continued)
```

```
DERV1Y(77) = -1.
С
C EFFECT OF PADIATION ON HE(V,J) CONCENTRATION
      SIGNL(I) IS TOTAL RATE OF EMISSION FROM HF(I) TO HF(I-1)
С
С
      PL = 0.
      KVAP = NOVAR
      00 180 I=1.3
      SIGNL(T) = 0.
      NO 180 J=1.15
      IF(NFLAG(1,J) .LF. 0) 50 TO 180
      KVAR = KVAR + 1
      IML = I + 16 + J - 9
      TMJ = T + 16 + J + 7
      ALP = ALPHA(T,J) + Y(1,KVAR)
      PL = PL + Y(1, KVAR) + WC(I, J)
      DER VIY (KVAF) = (ALPHA(I,J) - THGAIN) + 2.997925E+10 + Y(1,KVAR)
      DERVIY(IML) = DERVIY(IML) + ALP
      DERVIY(IMU) = DEPVIY(IMU) - ALP
      SIGNL(I) = SIGNL(I) + ALP
  180 CONTINUE
      SIGNL(4) = 0.
      \mathsf{DFPV1Y(1)} = \mathsf{DFRV1Y(1)} + \mathsf{SIGNL(1)}
      00 190 I = 2,4
  190 \quad OFPV1Y(I) = DEPV1Y(I) + SIGNL(I) - SIGNL(I-1)
C
C CALQULATE SUTFIT POWER
С
      HC+AVAGADEC NO. = 2.85912 CAL-CH/MOLE
С
      CONST = 2.85912 * THGAIN
      PL = PL + CONST
С
C TEMPERATURE DEPIVATIVE
2
      AI^{+} = Y(1,78)/100. + .5
      IT = IFTX(AIT)
      CVSUM = 2.981 * (HE + AR + Y(1,72)) + CVN2(IT) * N2 +
             CVH2(IT)*(Y(1,73) + Y(1,74) + Y(1,75)) +CVHF(IT)*(Y(1,1) +
     1
               Y(1,2) + Y(1,3) + Y(1,4) + Y(1,5) + Y(1,6) + Y(1,7)) +
     1
              CVSF6(IT) + SF6 + CVF(IT) + Y(1,76) + CVF2(IT) + Y(1,77)
     1
      ETHLPY = ((FHPYH(IT) + 52.102) - (EHPYF(IT) + 18.900)) #DERV1Y(72)
               +(EHPYF2(IT)) + DERV1Y(77) + (EHPYH2(IT)) + DERV1Y(73)
     1
                +(EMPYH2(IT) + 11.889) * DERV1Y(74)
     1
                +(FHPYH2(IT) + 23.112) * DERV1Y(75)
     1
                +(EHPYHF(IT) - 64.800) + DFPV1Y(1)
     1
                +(FHPYHF(IT) - 53.473) + DERV1Y(2)
     1
     1+(FHPYHF(IT) - 42.638) + DERV1Y(3) + (EHPYHF(IT) - 32.282) +
     10FPV1Y(4) + (EHPYHF(IT) - 22.392) * DEFV1Y(5) + (EHPYHF(IT) -
     1 12.959) * DERVIY(6) + (FHPYHF(IT) - 3.973) * DERVIY(7)
      FTHLPY = F^{T}HLPY + 1.F+3
      IF(FPP00.NF.0.)60 TO 12
      PIN=1.
      GO TO 11
   12 PIN=EPPCO#PA/EPPCDA
   11 CONTINUE
      PEPVIY(79) = - (PL + ETHLPY - PIN) / CVSUM
      IF(NVAP.LF.79) GC TO 230
      00 220 I = 79, NVAP
  220 TF(Y(1,T).LF.FLUX.AND.DERV1Y(I).LT.0.) DFPV1Y(I) = 0.
  230 CONTINUE
      PETURN
      FND
```

Table F.11. Subroutine FLASH

```
FUNCTION FLASH(T)
    DIMENSION CRPNT(2,100)
    DATA CRENT/-.8, C.0, 0.0, .3E-7, 2.0, .11E-6, 2.5, .15E-6, 2.6, .16E-6,
   12.57,.17F-6,2.7,.18E-5,2.7,.22E-6,2.68,.23F-6,2.65,.24E-6,2.6,
   1.25E-6,2.5,.26E-6,2.3,.28E-6,2.15,.29E-6,2.0,.3E-6,1.0,.36E-6,
   10.0,.43F-6.-2.0,.45E-6,-.38,.47E-6,-.6,.5E-6,-.84,.55E-6,-.92,
   1.58E-6,-.91,.6E-6,-.9,.62E-6,-.8,.65E-6,-.5,.7E-6,-.25,.75E-6,0.0,
   1.798-6/
    N= 28
    FLASH=0.
    IF(T.GF.CRPNT(2,N)) GO TO 200
    JC = 0
    00 100 I=1,N
    IF(T.GE.CRENT(2, I)) JC=JC+1
100 CONTINUE
    FLASH=(CRRHT(1,JC+1)-CRRNT(1,JC))*(T-CRRNT(2,JC))/(CRRNT(2,JC+1)-
   10RRNT(2, JC))+CPPNT(1, JC)
200 CONTINUE
    PETUCN
    END.
```

Table F.12. Subroutine DIFSUB^a

```
SUBFOUTINE DIFSUB(N, T, Y, SAVE, H, HMIN, HMAX, FPS, HF, YMAX, ERROR, KFLAG,
                       JSTART, MAXDER, PW, KEY)
    1
     DIMENSION Y (B,N), YMAX(N), SAVE(10,N), ERROP(N), PW(N),
               A(R), PERTST(7, 2, 3)
    1
     DATA PERTST /2.0,4.5,7.333,10.42,13.7,17.15,1.0,
                  2.0.12.0.24.0.37.89.53.33.70.08.87.97.
    1
                  3.0,6.0,7.167,12.5,15.98,1.0,1.0,
    1
                  12.0,24.0,37.89,53.33,70.08,87.97,1.0,
    1
                  1.,1.,0.5,0.1667,0.04133,0.008267,1.0,
    1
                  1.0,1.0,2.0,1.0,.3157,.07407,.0139/
    1
     DATA 4(2) / -1.0/
     IRFT =1
     KFLAG=1
     IF (JSTART.LE.0) 50 TO 140
 100 00 110 I = 1,N
       70 110 J= 1,K
110
         SAVE(J, I) = V(J, I)
     HOLD=HNEW
     IF (H.FQ.HOLD) GO TO 130
129
     RACUM=H/HOLD
     IRFT1=1
     50 TO 750
130
    NOOLDENO
     TOLD=T
     RACUM=1.0
     TE (JSTART.GT.P) GO TO 250
     GO TO 171
140 IF (JSTAPT.E0.-1) GO TO 160
     N2=1
     N3=N
     N1 = N^{#}10
     N2= N1 +1
     N4 = N##2
     N5 = N1 + "
     N6 = N5 + 1
     GALL DIFFUN (T,Y,SAVE(N2,1))
     00.150 I = 1.N
      111 = N1 + I
       Y(2,1) = SAVF(N11,1) +H
150
     HNFH = H
     K= 2
     GO TO 100
160 IF (NR.ER. NROLD) JSTART = 1
     T = TOLD
     NO= NOOLO
     K = NQ + 1
     GO TO 121
     IF (MF.EQ.0) 30 TO 180
170
     IF (NO.67.6) GO TO 190
     GO TO (221,222,223,224,225,226),NQ
     IF(NO.ST.7) GO TO 190
180
     GO TO (211,212,213,214,215,215,217),NO
190
     KFLAG = -2
     PFTUPN
     A(1) = -1.0
211
     GO TO 230
GO TO 230
```

| 213 | A(1) = -0.41666666666666667 |
|----------|--|
| 0.00 | A(3) = -0.7500000000000000000000000000000000000 |
| | A(4) = -1.1666666666666666667 |
| | |
| 214 | $\Lambda(1) = -0.37500000000000000000000000000000000000$ |
| - 1 - | A(3) = -0.9166666666666667 |
| | A(4) = -0.333333333333333333333333333333333333 |
| | A(5) = -0.0416666666666666667 |
| | a(3) = -3. |
| 215 | A(4) = -0 30861444444444444444444444444444444444444 |
| 615 | A(1) = -1, 0.16666666666666667 |
| | A(4) = -0.48644444444444444444444444444444444444 |
| | A(4) = -9.44001111111111111111111111111111111111 |
| | A(6) = -0.0000000000000000000000000000000000 |
| | GO TO 230 |
| 216 | A(1) = -0.32986111111111111111111111111111111111111 |
| 210 | A(3) = -1, 1416666666666666666666666666666666666 |
| | A(4) = -1.625000000000000000000000000000000000000 |
| | A(4) = -0.17708777777777777777777777777777777777 |
| | A(5) = -0.0250000000000000000000000000000000000 |
| | A(T) = -0.00138888888888888888888888888888888888 |
| | R(T) = -4.501338033003003003332 |
| 217 | A(1) = _0 3155010312160312 |
| 11 | A(3) = -1.23500000000 |
| | A(4) = -0.7518518518518519 |
| | A(5) = -0.2552083333333333333333333333333333333333 |
| | A(6) = -0.0486111111111111111111111111111111111111 |
| | |
| | |
| | A(7) = -N.NN4861111111111111111111111 |
| | A(8) = -0.0001984126984126984 |
| | 60 T 0.233 |
| 221 | A(1) = -1, 0000 |
| | GO TO 230 |
| 222 | A(1) = -0.5656666666666666666666666666666666666 |
| | A(3) = -0.333333333333333333333333333333333333 |
| | GO TO 230 |
| 223 | A(1) = -9.545454545454545454545454545454 |
| | A(3) = A(1) |
| | A(4) = -0.0909090909090909090909090909090909090 |
| | GO TO 230 |
| 224 | A(1) = -9.48000000000000000000000000000000000000 |
| | A(3) = -0.7000000000 |
| | A(4) = -0.2000000000000000 |
| | A(5) = -0.020000000000000000000000000000000000 |
| | GO TO 239 |
| 225 | A(1) = -0.437956204373562 |
| | A(3) = -0.8211578832116788 |
| | A(4) = -0.3102189781021898 |
| | A(5) = -0.05474452554744526 |
| | 4(6) = -0.0036496350364963504 |
| | GO TO 239 |
| 226 | A(1) = -0.4031632653061225 |
| | A(3) = -0.9206349206349206 |
| | $\Lambda(4) = -9.415656666666666667$ |
| | A(5) = -9.0992063492063492 |
| | A(5) = -0.0119047619047619 |
| | A(7) = -9.000566893424036282 |
| 230 | K = N() + 1 |
| . | IDuña = K |

```
Table F.12. (Continued)
```

```
MTYP = (4 - MF)/2
     END2 = .5/FLOAT(FO + 1)
     FN03 = .5/FLOAT(NQ + 2)
     EN01 = .5/FLOAT(10)
     PEPSH = FPS
     EUP = (PEPISI(NO, MTYP, 2) *PEPSH) **2
     E = (PERTST (ND, MTYP, 1) +PEPSH) ++2
     FOWN = (PFRTST(NO, HTYP, 3) + PEPSH) ++2
     IF (EDWN.ED.D) GC TO 730
     RND = FPS+FNO3/ FLOAT(N)
     IWEVAL = ME
241
     GO TO (250,630), JRET
     T = T + H
250
     30.260 J = 2.K
       70.250 J1 = J,K
         J_{2}^{2} = K - J_{1} + J - 1
         30.250 I = 1, N
             Y(J_2,I) = Y(J_2,I) + Y(J_2+1,I)
 250
     00 265 I=1, KFY
     TF(Y(1,I) .LT. C.) GO TO 440
 265 CONTINUE
     00 270 I = 1,N
?70
      FPROR(I) = 0.0
     00.430 L = 1,3
      CALL DIFFUN (T,Y,SAVE(N2,1))
     IF (TWEVAL.LT.1) GO TO 350
     IF (MF.ED. 7) 50 TO 310
     CALL PECEPU(T, Y, PW, N3)
     P = A(1) \neq H
     00 280 I = 1.84
      DM(I) = DM(I) +E
280
     M11 = M7 + 1
290
     N17 = N#111 - 1:3
     DO 300 I = 1, N12, N11
                                            4
300
       PW(I) = 1.0 + PW(I)
     IWEVAL = -1
     CALL MATINV(PW,N,N3,J1)
     IF (J1.GT.)) GO TO 350
     GO TO 440
310
     DO 320 I = 1, N
320
      SAVE(9,I) = Y(1,I)
     no 340 J = 1,N
       R = EPS*AMAX1(EPS, ABS(SAVE(9,J)))
       Y(1,J) = Y(1,J) + R
       0 = A(1) + H/2
       CALL DIFFUN(T,Y,SAVE(N6,1))
       330 I = 1, N
         N11 = T + (J-1) = N3
         M12 = M5 + I
         M17 = M1 + I
330
         PW(N11) = (SAVE(N12,1) - SAVE(N13,1)) + n
       Y(1,J) = SAVE(0,J)
340
     GO TO 290
     IF (MF.NE.0) 60 TO 373
350
     00 360 I = 1, N
       N11 = N1 + I
360
       SAVE(9,I) = Y(2,I) - SAVE(N11,1) + H
     GO TO 410
370 . 00 380 I= 1,N
```

```
N11 = N5 + I
       N12 = N1 + T
380
       SAVE(N11,1) = Y(2,1) - SAVE(N12,1) + H
      00 400 T = 1, M
       ) = n.n
       DO 390 J = 1,8
         N11 = I + (J-1) + N3
         N12 = N5 + J
390
         D = 0 + PW(N11) + SAVF(N12,1)
       SAVE(9, I) = 0
400
410
     NT = N
     00 420 I = 1.0
       Y(1,1) = Y(1,1) + A(1) + SAVE(9,1)
       Y(2,I) = Y(2,I) - SAVE(9,I)
       FRPOP(T) = EPPOR(I) + SAVE(3,I)
       TF ( A35(SAVE(9, I)).LE.(3ND*YMAX(I)))NT = NT - 1
    CONTINUE
420
     00 425 I=1.KEV
     IF(Y(1,I) .LT. 0.) GO TO 440
 425 CONTINUE
     IF (NT.LF.0) GO TO 493
     CONTINUE
430
440
    T = T - H
     IF ((H.LF. (HMIN+1.00001)). AND. ((IWEVAL - MTYP).LT.-1)) GO TO 460
     IF ((MF.EQ.0).0P.(IWEVAL.NE.0)) RACUM = PACUM * 0.2500
     IWEVAL = ME
     IRET1 = ?
   ....
     GO TO 751
    KELAS = -R
460
1690 FOR MAT(1H1/2E15.5,215,3E15.5////)
     PRINT 1690, H, HMIN, IWEVAL, MTYP, RACUM, HOLD, HMAX
470
     00 480 I = 1.N
       DO 480 J= 1,K
         Y(J,I) = SAVF(J,I)
480
     H = HOLD
     NO = NQOLD
     JETART = NO
     RETURN
490 D = N.N
     90500 I = 1, N
500
      0 = 0 + (FRROF(I)/YAX(I)) + 2
     IWFVAL = 0
     IF (0.6T.E) 50 TO 540
     IF (K.LT.3) GO TO 520
     10510 J = 3.K
       50510 I = 1,N
510
         Y(J,T) = Y(J,I) + A(J) + ERROR(I)
     KFLAG = +1
520
     HNEW = H
     IF (IDOUR.LF.1) GO TO 550
     10008 = 10003 - 1
     IF (IDOUR.GT.1) GO TO 700
     00 530 T = 1.N
530
       SAVE(10,T) = EFROR(I)
     60 TO 700
540
     KFLAG = KFLAG - 2
     IF (H.LE.(HMIN#1.00001)) GO TO 740
     T = TOLD
     IF (KFLAG.LE.-5) 60 TO 720
550
     PR2 = (D/5)**EN02*1.2
     PR3 = 1. F+20
```
Table F.12. (Continued)

```
JF ((ND.GE.MAXDEF).OR.(KFLAG.LE.-1)) GO TO 570
     n = 0.0
     00 560 I = 1,N
560 D=D+((FFPOP(T)-SAVE(10,I))/YMAX(I))**?
     PR3=(0/EUP) ##FN03#1.4
570 PR1 = 1.F+20
     TE (NQ.LE.1) GO TO 590
     D= 0.0
     00 580 I = 1,N
580
      n = n + (Y(K, I)/YMAX(I)) + ?
     PR1 = (C/FCWN) **EN01*1.3
590
     CONTINUE
     IF (PR2.LE.PP3) GO TO 650
     IF (PP3.LT. PP1) GO TO 660
    P = 1.0/AMAX1(PF1, 1.E-4)
600
     NEWO = NO - 1
     IDCUB = 10
610
     TF ((KFLAG.E).1).AND.(R.LT.(1.1))) GO TO 700
     D0 \ 6^{2}0 \ I = 1, N
621
       Y(NFWO+1, I) = FRROR(I) + A(K) / FLOAT(K)
    K = NEHC + 1
630
     TE (KELAS.E0.1) 60 TO 670
     RACUM = PACUMER
     IRFT1 = 3
     GO TO 759
640
    IF (NEWO.E0.NO) GO TO 250
     NO = NEWO
     GO TO 170
     TE (PP2.5T.PP1) GO TO 500
650
     MEWQ = NO
     R = 1.0/AMAX1(PF2, 1.E-4)
     GO TO 610
    R = 1.0/AMAX1(PF3,1.E-4)
660
     NFWO = NO + 1
     GO TO 617
670
     TRFT = 2
     R = AMIN1(R, 4MAX/ABS(H))
     H = H^{\mu}P
     HNEW = H
     IF (ND. FD. NEWD) GO TO 680
     NQ = NEWQ
     GO TO 170
680
     R1 = 1.0
     00 690 J = 2,K
       R1 = P1 + F
       00 690 I = 1,1
690
         Y(J,I) = Y(J,I) + P_1
     100Up = K
    00 710 I = 1,N
700
710
      YMAX(I) = AMAX1(YMAX(I), ABS(Y(1,I)))
     JSTART = NO
 RETUPN
720 IF (NO.FO.1) 50 TO 780
     CALL DIFFUN(T, Y, SAVE(N?, 1))
     R = 4/HOLD
     00.730 I = 1, N
     Y(1,I) = SAVE(1,I)
```

Table F.12. (Continued)

```
N11 = N1 + T
       SAVE(2,I) = HCLD*SAVE(N11,1)
730
       Y(2,I) = SAVE(2,I) + R
     NQ = 1
     KFLAG = 1
     GO TO 170
740 KFLAG = -1
     HNFW = H
     JSTART = NO
     RETURN
750 PACUM = AMAX1( APS(HMIN/HOLD), RACUM)
     RACUM = AMIN1(PACUM, ABS(HMAX/HOLD))
     R1 = 1.0
     00.760 J = 2.K
       P1 = R1#FACUM
       00 760 I = 1, M
        Y(J,I) = SAVF(J,I) + R1
 760
     H = HOLD#PACUM
     no 770 I = 1, N
 770
      Y(1,I) = SAVE(1,I)
     IDDUR = K
     GO TO (130,250,640), IRET1
 7AD KELAG = -4
     GO TO 470
     FND
```

,

^aThis algorithm is a modification of Algorithm 407 "DISFUB for Solution of Ordinary Differential Equations," by C. W. Gear, <u>Communications of the ACM</u>, 14, (3), (March 1971), pp. 185-190; copyright 1971, Association for Computing Machinery, Inc; used by permission.

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