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Numerical Formulation for Constant-Gain Chemical Laser Calculations*

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Equations are formulated for determining conditions in a chemically reacting gas situated inside an optical laser cavity. During lasing, the gain is held constant throughout the cavity as determined by a gain-equals-loss condition. For each vibrational level, a Boltzmann distribution for the rotational levels is assumed with lasing on each vibrational band at line center of the transition that has maximum gain. The final system consists of flow, chemical rate, and gain-equals-loss equations. Special numerical procedures for solving this system of coupled, nonlinear equations are described.

1. INTRODUCTION

The equations and numerical procedures are formulated for calculating conditions in a chemically reacting gas situated inside an optical laser cavity. The gas may be in motion, in which case it is treated as a steady, one-dimensional motion with lasing transverse to the direction of flow. The computer code [1] that performs these calculations also treats conditions in a time-dependent quiescent gas. The main assumptions are as follows:

1. A constant-gain method of calculation [1, 2] is used for the radiation. Inherent in this method are the approximation of a near Fabry–Perot cavity and the assumption of steady state for the stimulated emission. The short, initial transient period during which the spontaneous emission is selectively amplified in the medium is thus neglected.

2. The rotational populations for a given vibrational level are in a Boltzmann distribution at the translational temperature. This assumption applies when the characteristic time to achieve the distribution, usually the time for a few collisions, is short in comparison with a stimulated emission time. The stimulated emission

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time depends on the intensity level and thus varies from case to case. One important consequence of this assumption and the method of constant gain is that lasing occurs only on a single transition between any two adjacent vibrational levels. (Other transitions between the two vibrational levels have smaller gain and therefore do not satisfy the lasing threshold condition [3].) This transition is not fixed, but shifts to other rotational states during lasing.

The problem involves solution of a coupled system of ordinary differential equations and nonlinear algebraic equations. A complicating factor is the large number of discontinuities that occur during the course of the solution. A formulation of the equations suitable for efficient computation is given in Section 2, while the numerical procedures used in solution of the system are given in Section 3. Detailed solutions may be found in [3].

2. EQUATIONS

A. *Rate Equations*

The rate equations for nonlasing species are well known and need no discussion. For the lasing species they are written as

$$\rho V \frac{dn_i(v)}{dx} = \chi_{\mathrm{ch}}(v) + \chi_{\mathrm{rad}}(v) - \chi_{\mathrm{rad}}(v-1), \qquad v = 0, 1, \ldots, \tag{1}$$

where ρ is density, V is flow speed, $n_i(v)$ is the mole-mass ratio (mole/g) of species i in vibrational level v, and x is distance in the flow direction. $\chi_{\mathrm{ch}}(v)$ is the chemical production term given by

$$\chi_{\mathrm{ch}}(v) = \sum_r (\beta_{ri} - \alpha_{ri})(L_{fr} - L_{br}), \tag{2}$$

$$L_{fr} = k_{fr} \prod_j (\rho n_j)^{\alpha_{rj}}, \qquad L_{br} = k_{br} \prod_j (\rho n_j)^{\beta_{rj}}. \tag{3}$$

The parameters α_{rj} and β_{rj} are the stoichiometric coefficients of reactants and products, respectively, and k_{fr} and k_{br} are the forward and backward rate coefficients. The summation in Eq. (2) is over all reactions that alter $n_i(v)$. The quantity $\chi_{\mathrm{rad}}(v)$ accounts for the increase in $n_i(v)$ per unit volume due to lasing on the transition $(v + 1, J_{\max} + m) \rightarrow (v, J_{\max})$, where $J_{\max}$ is the rotational quantum number of the highest gain transition in the band and m is -1 for a P-branch transition and $+1$ for an R-branch transition. Similarly, $\chi_{\mathrm{rad}}(v-1)$ accounts for the decrease in $n_i(v)$ due to lasing from v to $v - 1$.

When lasing is not occurring between $(v+1)$ and v or between v and $(v-1)$, we have

$$dn_i(v)/dx = (1/\rho V)\, X_{\mathrm{ch}}(v), \tag{4}$$

and $n_i(v)$ is treated as a nonlasing species.

Equation (1) cannot be integrated directly as is done for the nonlasing species, since the $X_{\mathrm{rad}}(v)$ are unknown. To overcome this difficulty it is necessary to reformulate Eq. (1). This reformulation is expedited by introduction of two vectors $\delta(v)$ and $v^{(k)}$ such that

$$\delta(v) \equiv \begin{cases} 0, & \text{if } X_{\mathrm{rad}}(v) = 0, \\ 1, & \text{if } X_{\mathrm{rad}}(v) > 0, \end{cases} \tag{5}$$

where $v = 0, 1, \ldots, v_{\mathrm{fin}} - 1$. ($v_{\mathrm{fin}}$ is the highest vibrational level being considered). We adjoin to this vector the values $\delta(-1) = \delta(v_{\mathrm{fin}}) = 0$. The $v^{(k)}$ vector is defined as

$$0 \leqslant v^{(1)} < v^{(2)} < v^{(3)} < \cdots < v^{(2N)} \leqslant v_{\mathrm{fin}}, \tag{6}$$

where

$$\begin{aligned} &v^{(1)} \text{ is the smallest } v \text{ such that } \delta[v^{(1)}] = 1, \\ &v^{(2)} \text{ is the next larger } v \text{ such that } \delta[v^{(2)}] = 0, \\ &v^{(3)} \text{ is the next larger } v \text{ such that } \delta[v^{(3)}] = 1, \\ &v^{(4)} \text{ is the next larger } v \text{ such that } \delta[v^{(4)}] = 0, \end{aligned} \tag{7}$$

etc. This vector is $2N$ entries long. By means of the $\delta(v)$ we keep track of those vibrational bands that are lasing, while the $v^{(k)}$ keep track of a string of adjacent bands all of which are lasing.

One can readily show by writing out Eq. (1) with some of the $X_{\mathrm{rad}}(v)$ equal to zero that the following equations apply:

$$\begin{aligned} \sum_{v=v^{(1)}}^{v^{(2)}} \frac{dn_i(v)}{dx} &= \frac{1}{\rho V} \sum_{v=v^{(1)}}^{v^{(2)}} X_{\mathrm{ch}}(v), \\ \sum_{v=v^{(3)}}^{v^{(4)}} \frac{dn_i(v)}{dx} &= \frac{1}{\rho V} \sum_{v=v^{(3)}}^{v^{(4)}} X_{\mathrm{ch}}(v), \\ &\ \vdots \end{aligned} \tag{8}$$

There are N such equations, where N is defined by Eq. (6).

The $dn_i(v)/dx$ for the lasing species are finally determined by simultaneous solution of a set of equations consisting of Eq. (8), flow equations, and gain-equals-loss equations. These additional equations are discussed later.

Once values for dn_i/dx and $X_{\mathrm{ch}}(v)$ are known, we find the $X_{\mathrm{rad}}(v)$ by writing Eq. (1) as

$$\begin{aligned} X_{\mathrm{rad}}(0) &= -X_{\mathrm{ch}}(0) + \rho V(dn_i(0)/dx), \\ &\vdots \\ X_{\mathrm{rad}}(v) &= X_{\mathrm{rad}}(v-1) - X_{\mathrm{ch}}(v) + \rho V(dn_i(v)/dx). \end{aligned} \tag{9}$$

B. *Flow Conservation Equations*

The equations of state, momentum, and continuity are unaltered from the final form given for them in [1]. For completeness we repeat them here:

$$\frac{1}{T}\frac{dT}{dx} + \frac{1}{\rho}\frac{d\rho}{dx} - \frac{1}{p}\frac{dp}{dx} = \Lambda_2, \tag{10}$$

$$\frac{1}{A}\frac{dA}{dx} + \frac{1}{\rho}\frac{d\rho}{dx} - \Gamma_2\frac{1}{p}\frac{dp}{dx} = 0, \tag{11}$$

where T is temperature, p is pressure, A is flow area, and V has been eliminated by means of the continuity equation. The quantities Γ_2 and Λ_2 are defined in terms of the molecular weight W and the universal gas constant R as

$$\Gamma_2 \equiv RT/WV^2, \tag{12}$$

$$\Lambda_2 \equiv -W\sum\frac{dn_i}{dx}. \tag{13}$$

Finally, the quantity $\sum(dn_i/dx)$ can be written as

$$\sum\frac{dn_i}{dx} = \sum_{\substack{\text{nonlasing}\\ \text{species}}}\frac{dn_i}{dx} + \frac{1}{\rho V}\sum_{v=0}^{v_{\mathrm{fin}}} X_{\mathrm{ch}}(v), \tag{14}$$

since all nonzero X_{rad} terms cancel when Eq. (1) is summed over v.

C. *Energy Equation*

The energy equation can be written for a unit volume of gas in the form

$$\rho\frac{dh}{dt} - \frac{dp}{dt} = -\sum_{v=0}^{v_{\mathrm{fin}}-1}\frac{dP(x;v)}{d\,\mathrm{Vol}}, \tag{15}$$

where t is time and P is lasing output power. The specific enthalpy h is

$$h = \sum H_i n_i, \tag{16}$$

where $H_i(T)$ is the molar enthalpy of species i. Equation (15) is written for a differential volume, which equals $A\,dx$. The summation on the righthand side represents the laser energy that leaves this volume per unit time.

After some straightforward manipulation and using the steady-flow relation $d(\ )/dt = V[d(\ )/dx]$, we obtain for the energy equation

$$\Gamma_1 \frac{1}{T}\frac{dT}{dx} - \frac{1}{p}\frac{dp}{dx} = \Lambda_1 - \frac{1}{pVA}\sum_{v=0}^{v_{\text{fin}}-1} \frac{dP(x;v)}{dx}, \tag{17}$$

where

$$\Gamma_1 \equiv \frac{W}{R}\sum n_i \frac{dH_i}{dT}, \tag{18}$$

$$\Lambda_1 \equiv -\frac{W}{RT}\sum H_i \frac{dn_i}{dx}. \tag{19}$$

For later convenience, we rewrite Λ_1 as

$$\Lambda_1 = \Lambda_{1\,\text{mod}} - \frac{W}{RT}\sum_{v=0}^{v_{\text{fin}}} H_i(v)\frac{dn_i(v)}{dx}, \tag{20}$$

$$\Lambda_{1\,\text{mod}} \equiv -\frac{W}{RT}\sum_{\substack{\text{nonlasing}\\ \text{species}}} H_i \frac{dn_i}{dx}. \tag{21}$$

The derivative of the output power $P(x;v)$ for transition $(v+1, J+m) \rightarrow (v, J)$ is given by [1]

$$dP(x;v)/dx = hcN_A A(x)\,\omega_c(v, J_{\max}, m)\,\chi_{\text{rad}}(v), \qquad v = 0, 1, \ldots, \tag{22}$$

where h is Planck's constant, c is the speed of light, N_A is Avogadro's number (since χ_{rad} is in molar units), and ω_c is the wavenumber of the transition in cm^{-1}. Define $\bar{K}$ as

$$\bar{K} \equiv hcN_A \frac{\rho}{p} = hcN_A \frac{W}{RT}. \tag{23}$$

By substituting $\bar{K}$ and Eqs. (20) and (22) into Eq. (17), we obtain the final form for the energy equation

$$\Gamma_1 \frac{1}{T}\frac{dT}{dx} - \frac{1}{p}\frac{dp}{dx} + \bar{K}\sum_{v=0}^{v_{\text{fin}}} \frac{dn_i(v)}{dx}\left[\frac{1}{hcN_A} H_i(v) + \delta(v)\sum_{j=v}^{v^{(k+1)}-1} \omega_c(j)\right]$$

$$= \Lambda_{1\,\text{mod}} + \frac{\bar{K}}{\rho V}\sum_{v=0}^{v_{\text{fin}}} \delta(v)\,\omega_c(v)\sum_{j=v^{(k)}}^{v} \chi_{\text{ch}}(j). \tag{24}$$

The two j-sums need be computed only when $\delta(v) = 1$. In these sums, therefore, k is an odd integer and $v^{(k)} \leqslant v < v^{(k+1)}$. With this in mind, we see that the double sum on the lefthand side stems from the relation

$$\sum_{v=0}^{v_{\mathrm{fin}}} \delta(v)\, \omega_c(v) \sum_{j=v^{(k)}}^{v} \frac{dn_i(j)}{dx} = \sum_{v=0}^{v_{\mathrm{fin}}} \frac{dn_i(v)}{dx}\, \delta(v) \sum_{j=v}^{v^{(k+1)}-1} \omega_c(j). \tag{25}$$

D. *Flow Model Equation*

The flow model is controlled by the identity

$$a_1 \frac{1}{T}\frac{dT}{dx} + a_2 \frac{1}{A}\frac{dA}{dx} + a_3 \frac{1}{\rho}\frac{d\rho}{dx} + a_4 \frac{1}{p}\frac{dp}{dx} = b. \tag{26}$$

Its use is best described by an example. If the flow model is defined by specification of density as a function of distance, the program sets $a_1 = a_2 = a_4 = 0$, $a_3 = 1$, and $b = (1/\rho)(d\rho/dx)$. Including Eq. (26) in the set of simultaneous equations to be solved avoids the need to define a separate set of equations for each flow model.

E. *Gain Coefficient*

The gain coefficient α, which is the relative change in the intensity I, is given by

$$\begin{aligned} \alpha(v, J, m) &= (1/I)(dI/dx) = (hN_A/4\pi)\, \omega_c(v, J, m)\, \phi_c \rho B(v, J, m) \\ &\quad \times \{[(2J + 1)/(2J + 1 + 2m)]\, n_i(v + 1, J + m) - n_i(v, J)\}, \end{aligned} \tag{27}$$

where $B(v, J, m)$ is the Einstein absorption coefficient. The mole–mass ratio for the rotational population of the lasing species $n_i(v, J)$ is related to the vibrational population by means of the Boltzmann equation

$$n_i(v, J) = n_i(v) \frac{2J + 1}{Q_{\mathrm{rot}}^{(v)}} \exp\left(-\frac{hc}{k}\frac{E_{v,J}}{T}\right), \tag{28}$$

where $Q_{\mathrm{rot}}^{(v)}$ and $E_{v,J}$ (in cm^{-1}) are the rotational partition function and the rotational energy, respectively, and k is Boltzmann's constant. The line profile ϕ_c at wave number ω_c is given by

$$\phi_c = (\ln 2/\pi)^{1/2}\, [K(0, y)/\alpha_{\mathrm{DP}}(v, J, m)], \tag{29}$$

where α_{DP} is the Doppler half-width, in wavenumber units, at half the peak intensity and is given by

$$\alpha_{\mathrm{DP}}(v, J, m) = \left(\frac{2 \times 10^7 N_A k \ln 2}{c}\right)^{1/2} \omega_c(v, J, m)(T/W^*)^{1/2}. \tag{30}$$

W^* is the molecular weight of the lasing molecule. $K(0, y)$ is the value of the line profile at line center described by the Voigt function [5]

$$K(0, y) = e^{y^2}[1 - \operatorname{erf}(y)], \tag{31}$$

where

$$y = (\ln 2)^{1/2}\, [\alpha_{\mathrm{LR}}(v, J)/\alpha_{\mathrm{DP}}(v, J, m)], \tag{32}$$

and α_{LR} is the Lorentz half-half width [6].

F. *Gain-Equals-Loss Condition*

We define operationally the terms threshold, cutoff, and J-shift. By threshold on v we mean the first time any rotational transition $(v + 1) \rightarrow v$ lases. Cutoff on v means that all rotational transitions $(v + 1) \rightarrow v$ have stopped lasing, i.e., $\chi_{\mathrm{rad}}(v) = 0$. Finally, J-shifting means that lasing has shifted from the $(v + 1, J + m) \rightarrow (v, J)$ transition to an adjacent rotational transition $(v + 1, J + m \pm 1) \rightarrow (v, J \pm 1)$. None of the locations where threshold, J-shifts, or cutoffs occur are known beforehand.

The quantities $J_{\max}$ and $v_{\max}$ are defined as follows. From the array,

$$\begin{array}{c} R\text{-branch} \leftarrow | \rightarrow P\text{-branch} \\ \ldots, \alpha(v, 1, 1), \alpha(v, 0, 1), \alpha(v, 1, -1), \alpha(v, 2, -1), \ldots, \end{array} \tag{33}$$

we locate the unique maximum designated as $\alpha(v, J_{\max}, m)$. Frequently, the R-branch is excluded from this search, since one can show that for most diatomics the maximum gain transition is in the P-branch [3].

After the $\alpha(v, J_{\max}, m)$, $v = 0, 1, \ldots$, array is completed, we search this array for the largest α, designated as $\alpha(v_{\max}, J_{\max}, m)$. This search is done only over those v where no $(v + 1) \rightarrow v$ transition is lasing. Our purpose is to determine the next transition to go through threshold and the location where this occurs.

The gain-equals-loss condition is written as [1, 2]

$$r_0(x)\, r_L(x) \exp[2L\alpha(v, J_{\max}, m)] = 1, \qquad v = 0, 1, \ldots . \tag{34}$$

The specified reflectivities of the two mirrors are r_0 and r_L, and L is the length of active medium between the mirrors and is assumed constant.

Equation (34) appears in the literature in different forms and with different names. For example, it is sometimes referred to as a saturation condition [7], since it forces the gain to have a value generally very different from a zero-power value. It can also be considered as a steady-state relation for the radiation [3]. We refer to Eq. (34) as a gain-equals-loss equation because the exponential gives the round-trip gain in the intensity, while the product $r_0 r_L$ gives the attenuation in the intensity at the two mirrors that just balances the round-trip gain.

We wish to re-express Eq. (34) as a differential equation, since it will be used in a system of equations that is linear in the derivatives. We first combine Eqs. (27)–(31) to obtain

$$\alpha(v, J, m) = \left[\frac{h^2c^2N_A}{32 \times 10^7\pi^3 k}\frac{W^*}{T}\right]^{1/2} \rho B(v, J, m)(2J + 1)$$
$$\times \left[\frac{n_i(v + 1)}{Q_{\text{rot}}^{(v+1)}} \exp\left(-\frac{hc}{k}\frac{E_{v+1,J+m}}{T}\right) - \frac{n_i(v)}{Q_{\text{rot}}^{(v)}} \exp\left(-\frac{hc}{k}\frac{E_{v,J}}{T}\right)\right]. \tag{35}$$

Equation (35) is strictly valid only for a Doppler line profile. The more general Voigt profile leads to excessively complicated results when $\alpha(v, J, m)$ is differentiated. For a gas at low pressure, the line profile at line center is accurately given by a Doppler profile and the error in the above approximation is negligible. Even in those calculations performed to date at a high pressure (one atmosphere or more), where the transition has a Lorentz profile, the variation in gain from the correct Voigt value has been less than 5 %.

We next combine Eqs. (34) and (35) to obtain

$$A_1(v) = A_2(v) + \left[\frac{32 \times 10^7\pi^3 k}{h^2c^2N_A}\frac{T}{W^*}\right]^{1/2} \frac{\ln(r_0 r_L)}{2L\rho B(v, J_{\text{max}}, m)(2J_{\text{max}} + 1)}, \tag{36}$$

where A_1 and A_2 are

$$A_1(v) \equiv \frac{\delta(v)\, n_i(v)}{Q_{\text{rot}}^{(v)}} \exp\left(-\frac{hc}{k}\frac{E_{v,J}}{T}\right), \tag{37}$$

$$A_2(v) \equiv \frac{\delta(v)\, n_i(v + 1)}{Q_{\text{rot}}^{(v+1)}} \exp\left(-\frac{hc}{k}\frac{E_{v+1,J_{\text{max}}+m}}{T}\right). \tag{38}$$

The $\delta(v)$ coefficient is inserted in both expressions for convenience. We now differentiate Eq. (36) to obtain our final form for the gain-equals-loss equation

$$\left\{\left[\frac{hcE_{v,J_{\text{max}}}}{kT} - C(v, T) - \frac{1}{2}\right] A_1(v)\right.$$
$$\left. - \left[\frac{hcE_{v+1,J_{\text{max}}+m}}{kT} - C(v + 1, T) - \frac{1}{2}\right] A_2(v)\right\} \frac{1}{T}\frac{dT}{dx}$$
$$+ [A_1(v) - A_2(v)]\frac{1}{\rho}\frac{d\rho}{dx} + \frac{A_1(v)}{n_i(v)}\frac{dn_i(v)}{dx}$$
$$- \frac{A_2(v)}{n_i(v + 1)}\frac{dn_i(v + 1)}{dx} = [A_1(v) - A_2(v)]G, \qquad v = 0, 1, \ldots, \tag{39}$$

where

$$C(v, T) \equiv \frac{d \ln Q_{\text{rot}}^{(v)}}{d \ln T}, \qquad G = \frac{1}{\ln(r_0 r_L)} \frac{d \ln(r_0 r_L)}{dx}. \tag{40}$$

We conclude this section by noting that our formulation is applicable to a quiescent gas if we simply set $x = t$, $A = 1$, and $V = 1$.

3. NUMERICAL PROCEDURES

A. *Integration Method*

We use a standard, fourth-order, Runge–Kutta method for the integration. The maximum allowable step size B_K is determined by the chemistry [8] and is used whenever lasing is not occurring. We refer to B_K as the maximum allowable step size because the actual integration step size is frequently smaller. The need for a smaller step size is a consequence of the discontinuities at threshold, J-shift, and cutoff points. The step size is adjusted so that these discontinuities occur between integration steps, not during them.

Unlike some methods, Runge–Kutta does not require data from previously computed steps. Hence, discontinuities are easily handled. For this reason and because of the accuracy, modest storage requirement, and, most importantly, the ease with which the step size can be altered by an arbitrary amount, the Runge–Kutta method is preferable for calculations of this type.

B. *The Nonlasing A-Matrix*

At the start of a calculation, the gain coefficients $\alpha(v, J, m)$ are computed and we test the inequality

$$r_0 r_L \exp[2L\alpha(v_{\max}, J_{\max}, m)] < 1. \tag{41}$$

If it is satisfied, then lasing has not yet occurred. The integration during nonlasing periods is the simpler case and, therefore, is discussed separately at this time.

The derivatives dn_i/dx are computed from Eq. (4). Since this is a nonlasing situation, all $\chi_{\text{rad}}(v) = 0$ and all $\delta(v) = 0$. The four Eqs. (10), (11), (17), and (26) are set up in the following format:

$$\begin{bmatrix} 1 & 0 & 1 & -1 \\ 0 & 1 & 1 & -\Gamma_2 \\ \Gamma_1 & 0 & 0 & -1 \\ a_1 & a_2 & a_3 & a_4 \end{bmatrix} \begin{bmatrix} \dfrac{1}{T} \dfrac{dT}{dx} \\ \dfrac{1}{A} \dfrac{dA}{dx} \\ \dfrac{1}{\rho} \dfrac{d\rho}{dx} \\ \dfrac{1}{p} \dfrac{dp}{dx} \end{bmatrix} = \begin{bmatrix} A_2 \\ 0 \\ A_1 \\ b \end{bmatrix}, \tag{42}$$

from which the derivatives of T, A, ρ, and p are easily solved. This procedure is continued until threshold is encountered. For convenience, we have named this form the A-matrix.

C. *Detection of Threshold, J-Shift, Cutoff*

Each time a transition between v and $v + 1$ reaches threshold, there is a discontinuous change in the derivative of $n_i(v + 1)$ and of $n_i(v)$ due to the inception of lasing on this transition. Consequently, the structure of the A-matrix, discussed shortly, will change; the A-matrix, therefore, must be reformulated and an updated set of $dn_i(v)/dx$ must be calculated before the Runge–Kutta integration can proceed.

At each integration step, the $\alpha(v, J_{\max}, m)$ array is checked for each v to determine whether the $J_{\max}$ for that transition has changed from its value at the preceding step. If such a change has occurred, the derivatives of $n_i(v)$ and $n_i(v + 1)$ show discontinuous changes and must be recalculated, and the A-matrix must be updated, before the integration can continue.

Prior to each integration step, all transitions lasing on the previous step must be checked for cutoff. If a $(v + 1) \rightarrow v$ transition was lasing during the previous step but now shows a $\chi_{\text{rad}}(v) \leqslant 0$, cutoff has occurred.

D. *Step Size Control*

During nonlasing periods, the step size is computed solely on the basis of numerical stability as affected by the chemistry. During lasing periods, frequent encounters with new transitions, J-shifts, and cutoffs make orthodox methods unsatisfactory. Even in that portion of the integration antecedent to lasing, additional control must be exercised so that the threshold location is situated between integration steps. These controls are maintained at each step by computation of alternative step sizes on the basis of discontinuity and other limiting criteria and selection of the smallest of the alternatives for use in the integration. Any negative Δx is discarded in this selection process. Candidate step sizes are calculated with respect to numerical stability, threshold, J-shift, and cutoff.

For previously nonlasing transitions, threshold occurs when inequality (41) is no longer satisfied. We can account for any upcoming discontinuity due to a new threshold by determining the largest $\alpha(v, J_{\max}, m)$ from the nonlasing transitions and calculating, by a modified linear extrapolation, the step size necessary for that gain coefficient to reach the critical value $-(\ln r_0 r_L) + 2L$. Simple linear extrapolation, which initially was used, was found to be very inaccurate for predicting this location. (This method would frequently result in a gain value well above that at threshold). The difficulty was overcome by use of an under-relaxation/over-relaxation technique; namely, the linearly extrapolated value for step size is multiplied by a coefficient whose value is either 0.6, 0.9, or 1.01. The coefficient 0.6 is used in the calculation of the candidate step size at each step

$$
\begin{array}{c|ccccccc}
\text{Eq.} \backslash \text{Variable} & T & A & \rho & p & n_i(0) & n_i(1) & n_i(2) \\
\hline
(24) & \Gamma_1 & 0 & 0 & -1 & a_{15} & a_{16} & a_{17} \\
(10) & 1 & 0 & 1 & -1 & 0 & 0 & 0 \\
(11) & 0 & 1 & 1 & -\Gamma_2 & 0 & 0 & 0 \\
(26) & a_1 & a_2 & a_3 & a_4 & 0 & 0 & 0 \\
(4) & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
(8) & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
(39) & a_{71} & 0 & [A_1(1) - A_2(1)] & 0 & 0 & \frac{A_1(1)}{n_i(1)} & -\frac{A_2(1)}{n_i(2)}
\end{array}
\begin{pmatrix}
\frac{1}{T}\frac{dT}{dx} \\
\frac{1}{A}\frac{dA}{dx} \\
\frac{1}{\rho}\frac{d\rho}{dx} \\
\frac{1}{p}\frac{dp}{dx} \\
\frac{dn_i(0)}{dx} \\
\frac{dn_i(1)}{dx} \\
\frac{dn_i(2)}{dx}
\end{pmatrix}
=
\begin{pmatrix}
\Lambda_{1\mathrm{mod}} + \frac{\overline{K}}{\rho V}\omega_c(1)[\chi_{ch}(1) + \chi_{ch}(2)] \\
\Lambda_2 \\
0 \\
b \\
\frac{1}{\rho V}\chi_{ch}(0) \\
\frac{1}{\rho V}[\chi_{ch}(1) + \chi_{ch}(2)] \\
[A_1(1) - A_2(1)]G
\end{pmatrix}
$$

where

$$a_{71} = \left[\frac{hcE_{1,J_{\max}}}{kT} - C(1,T) - \frac{1}{2}\right]A_1(1) - \left[\frac{hcE_{2,J_{\max}+m}}{kT} - C(2,J) - \frac{1}{2}\right]A_2(2)$$

$$a_{15} = \overline{K}\left[\frac{1}{hcN_A}H_i(0) + \omega_c(1)\right]$$

$$a_{16} = \overline{K}\left[\frac{1}{hcN_A}H_i(1) + \omega_c(1)\right]$$

$$a_{17} = \overline{K}\left[\frac{1}{hcN_A}H_i(2) + \omega_c(1)\right]$$

FIG. 1. The Lasing A-Matrix; $\delta(-1) = \delta(0) = 0, \delta(1) = 1, \delta(2) = 0$.

until such a candidate becomes selected as the Δx for that step. Once this happens, the coefficient 0.9 is then used for computing the candidate Δx at the following step; if this candiate also becomes selected, then the coefficient 1.01 is used for each successive candidate Δx until the sequence is broken by determination of the integration step size by some means other than imminent threshold. Anytime the sequence is broken, the coefficient reverts to the value 0.6. In addition, it has been found necessary to calculate a step size for threshold on the adjacent rotational transitions to cover those situations in which a J_{max}-shift simultaneously may occur. The minimum Δx so determined becomes a candidate step size.

A similar treatment is applied to $\alpha(v, J_{\text{max}} \pm 1, m)$ after threshold so that a step size dependent upon J-shifting can be calculated. The Δx necessary for each $\alpha(v, J_{\text{max}} \pm 1, m)$ to equal $\alpha(v, J_{\text{max}}, m)$ is computed. Again it is necessary to supplement the linear extrapolation with an under-relaxation/over-relaxation technique. The J-shift candidate step size is calculated by multiplication of the linearly extrapolated value by the coefficient 0.8 at each step until such a candidate becomes selected as the Δx for that step. Once this happens, the coefficient 1.01 is then used in computation of the candidate Δx at each successive step until the sequence is broken by determination of the integration step size by some means other than an approaching J-shift. When the sequence is broken, the coefficient reverts to the value 0.8.

A candidate step size is also computed on the basis of each lasing transition reaching cutoff. This is determined via conventional linear extrapolation, which is sufficiently accurate in this case.

E. *The Lasing A-Matrix*

Once lasing begins, it is advantageous to add additional $v_{\text{fin}} + 1$ equations to the nonlasing A-matrix in order to solve for the $dn_i(v)/dx$ simultaneously with dT/dx, dA/dx, dp/dx, and $d\rho/dx$.

The first four rows of the matrix are Eqs. (24), (10), (11), and (26), as shown in Fig. 1. Equation (4) is used whenever $\delta(v) + \delta(v - 1) = 0$. Since $N = 1$, we require only one equation of the form Eq. (8). Finally, there are $\sum \delta(v) = 1$ Eqs. (39), which complete the A-matrix. Solution of the matrix equation then yields the derivatives that are numerically integrated.

REFERENCES

1. G. EMANUEL, W. D. ADAMS, AND E. TURNER, "Resale-1: A Chemical Laser Computer Program," TR-0172(2776)-1, The Aerospace Corp. 1972.
2. J. R. AIREY, *J. Chem. Phys.* **52** (1970), 156–167.
3. G. EMANUEL, *J. Quant. Spectr. Radiative Transf.* **11** (1971), 1481–1521.

4. G. Emanuel, N. Cohen, and T. A. Jacobs, "Theoretical Performance of an HF Chemical CW Laser," TR-0172(2776)-2, The Aerospace Corp. (1972).
5. B. H. Armstrong, *J. Quant. Spectr. Radiative Transf.* 7 (1967), 61–88.
6. S. S. Penner, "Quantitative Molecular Spectroscopy and Gas Emissivities," Addison-Wesley, Reading, MA, 1959.
7. W.C Marlow, *J. Appl. Phys.* **41** (1970), 4019–4022.
8. G. Emanuel and H. J. Vale, A generalized major product solution method for nonequilibrium thermochemical problems, *in* "The Performance of High Temperature Systems" (G. S. Bahn, Ed.) Vol. 2, p. 497, Gordon and Breach, New York, 1969.