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A MODEL FOR THE CW POWER OUTPUT
OF THE HF CHEMICAL LASER

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ABSTRACT

A radiation model is presented for inclusion in hydrodynamics codes calculating steady-state chemical lasing conditions. The model assumes that if sufficient gain exists for lasing to occur, then P-branch lasing occurs for $3 \rightarrow 2$, $2 \rightarrow 1$ and $1 \rightarrow 0$ transitions at the (local) J value corresponding to maximum zero power gain. For simplicity, all HF states with $v > 3$ are ignored. The theory yields the local and total power output, the local specific intensity of the radiation field and the local distribution of the HF population among the vibrational states. Very crude predictions could be obtained for the spectral distribution of the emitted radiation, although the theory is not well suited to that purpose.

I. INTRODUCTION

The model presented here for the CW chemical laser is intended for incorporation as an "optics package" for the RICE¹ program, although it is not specifically constrained to that application. This work relies heavily on several studies of Emanuel^{2,3,4} and is especially indebted to his pioneering article² clarifying the lasing phenomenology and demonstrating the applicability of a highly idealized model of the lasing process. The present model gives a slightly more complete description of the physics of the lasing process than is provided by Emanuel's two closed-form solutions.^{2,3} However, the principal improvement is provided by the treatment of the strong spatial nonuniformities in species concentrations and in temperature which occur¹ in the direction of laser propagation. Because of these spatial nonuniformities, the present model provides a closed-form solution only in certain approximation. Strictly, it is necessary to solve for the specific intensity of the radiation for each $v+1 \rightarrow v$ transition and for the concentration of each vibrational state of HF self-consistently.

The "optics package" provides the equations for this purpose, a first approximation to a solution of the equations and a prescription for the iterative solution of the equations.

The model assumes that each volume element of the gas either does not lase or, if the zero power gain exceeds the threshold gain, lases at the (P-branch) vibrational-rotational transition with maximum zero power gain. No attempt is made to follow the evolution of the dominant lasing modes. Instead, it is simply assumed that all three transitions $3 \rightarrow 2$, $2 \rightarrow 1$ and $1 \rightarrow 0$ lase at the single J value determined by the maximum zero power gain. All vibrational states with $v > 3$ are ignored throughout the calculation. It is assumed that all vibrational-rotational lines are Doppler broadened and all gains are computed at line center. This has the effect of assuming that for each $v+1 \rightarrow v$ transition lasing occurs on the single Fabry-Perot longitudinal mode closest to line center or that, if multiple modes are excited, none is very far from line center. All hole burning effects are ignored. Some spectral information is contained in the model; for at each

point at which lasing occurs a single J value is excited and this J value changes with location in the gas. However, this change in J value is discontinuous and no provision is made for the lasing on several J values and the shifting of excited longitudinal modes which is typical of transition regions for J shifting in actual lasers. The model is, of course, most suited to describe low-pressure ($< 1\text{-atm}$) lasers.

The model adapts readily to any desired level of treatment of vibrational-translation and vibrational-vibrational HF energy transfer reactions, since the mathematical formulation does not depend on the specific form taken for the "chemistry" reactions. The model assumes the rigid rotator approximation for the HF energy levels, but, at the price of some algebraic complexity, this restriction could be removed. Similarly, the restriction to $v \leq 3$ could be removed (and should be removed for applications in which the $\text{H} + \text{F}_2 \rightarrow \text{HF} + \text{E}$ reaction is of importance). The matrix elements connecting the upper and lower lasing states are allowed to depend on both quantum numbers J and v . This dependence affects the populations required for threshold gain by factors of two or three. The threshold gain condition provides a set of integral constraints on the vibrational populations of HF in the presence of spatial inhomogeneities. It is essential to the easy applicability of the model to replace these integral constraints by algebraic constraints on the total HF vibrational populations. This replacement requires a certain approximate treatment of the temperature profile which is basic to the model.

II. THE FLOW CONFIGURATION

The primary hydrodynamic flow is in the x -direction. Hydrogen gas and dissociated fluorine gas are admitted into the system at supersonic velocities through a series of rectangular nozzles at $x=0$. Mixing of the fluids occurs in the z -direction and hydrodynamic variables acquire a z -dependence. However, boundary layer effects, which give rise to a y -dependence of flow quantities, will be ignored.

Plane parallel mirrors are assumed to be placed adjacent to the gas flow. This will be an adequate modeling of the physical situation, provided that any region existing between the gas and the mirrors

has negligible losses and provided that the laser approximates a Fabry-Perot cavity. Mirror losses and edge effects are also ignored. The radiation path is thus taken to be strictly in the z -direction, and the region of the gas in which possible lasing occurs is taken to be

$$x_0 < x < x_0 + d ,$$

$$0 < y < H ,$$

and

$$0 < z < L . \quad (1)$$

The configuration is depicted in Fig. 1.

III. RADIATIVE TRANSPORT IN THE SYSTEM

The equations describing radiative transport have been written down many times in the extensive literature on the subject, but the notation and units are far from standard, even in the portion of the literature relevant to CW lasers. Also, occasional numerical errors occur in the formulas for the constants defining the theory. Thus we will give here a consistent set of equations defining the theory in cgs units before applying the theory to

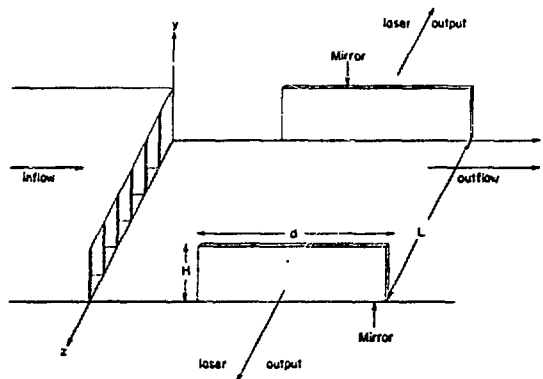


Fig. 1. The flow geometry for CW operation of the HF chemical laser. Basic hydrodynamic flow is in the x -direction with mixing in the z -direction. Radiation path is the z -direction.

the calculation of laser power output. We will always work in the framework of radiation transport theory. That is, no phase information is used in the evaluation of the radiation field, even though the field is coherent. The notation will follow Gilles and Vincenti⁵ as far as possible.

The basic quantity of the theory is the specific intensity $I_{\nu}(\vec{r}, \vec{\Omega})$ of a steady-state radiation field and is given here in units of ergs cm^{-2} - sterad⁻¹. No attempt is made to follow the time evolution of the lasing modes. The ambiguity of which of the possible lasing modes are present in the steady-state radiation field is settled by simply postulating a mode structure which is not unreasonable but is underived. However, the amplitudes of the permitted modes are determined self-consistently from the transport equation and the chemical rate equations.

We denote by B_{LU} the Einstein coefficient for absorptions per unit time per atom per unit solid angle. In each absorption an HF molecule is transferred from a lower lasing state $L = (v, J)$ to an upper lasing state $U = (v+1, J-1)$. We assume lasing always occurs on the P-branch. Then if W denotes the upward transition probability per unit time per steradian for an HF molecule in the L-state, we have

$$W = B_{LU} I_{\nu} \quad (2)$$

With the above conventions the numerical value of the Einstein coefficient is given by

$$B_{LU} = \left(\frac{8\pi^3}{3h^2 c} \right) \left(\frac{J}{2J+1} \right) \left| M_{v, J}^{v+1, J-1} \right|^2 \quad (3)$$

where h denotes Planck's constant, c the velocity of light and $M_{v, J}^{v+1, J-1}$ the irreducible part (independent of magnetic quantum number) of the dipole length matrix element of the transition. The above definition of B_{LU} is certainly not the only one in the literature. In particular, it agrees with the conventions of Thoenes and Ratliff⁶ and differs by a factor of $4\pi \times 10^{-7}$ from those of Emanuel.⁴ We note in passing that the cgs units for B_{LU} are $\text{cm}^2 \text{erg}^{-1} \text{sec}^{-1}$.

Numerical values are obtained from a calculation of Meredith quoted by Emanuel.² Because the calculation is unpublished, because the calculational model is not precise, and because fine details of the matrix element's value should not significantly affect the lasing population, the fit to the calculation is rather crude. A more refined fit to different data is provided by Thoenes and Ratliff.⁶ The features of the calculation that it was considered desirable to model were roughly linear variations of $|M|^2$ with J and with v , since these will cause factors of two or more variations in the vibrational populations. Thus the dipole length matrix element is specified by

$$\left| M_{v, J}^{v+1, J-1} \right|^2 = (1 + 0.06J)(v+1) \times 10^{-38} \text{ erg cm}^3 \quad (4)$$

This formula agrees reasonably well with the Meredith calculations which are reported for $v \leq 2$ and with the fit of Thoenes and Ratliff.⁶

We will assume that the lasing lines are Doppler broadened and that the induced emission line shape η_{UL} is equal to the absorption line shape $\phi_{LU}(v)$. The former assumption is well satisfied under usual (~ 1 Torr) CW lasing conditions, but will be seriously violated at atmospheric pressures. The latter assumption amounts to asserting that lasing occurs on a Fabry-Perot mode sufficiently close to line center that the differing shapes⁵ of η_{UL} and ϕ_{LU} may be ignored. In any event, the correct Doppler broadened absorption line shape at line center ν_0 satisfies

$$\nu_0 \phi(\nu_0) = \left(\frac{MWc^2}{2\pi kT} \right)^{1/2} \quad (5)$$

which differs by a factor of $\sqrt{\ln 2}$ from some values^{2,3} reported in the literature. In Eq. (5) M denotes the proton mass, W the molecular weight of the lasing molecule, k the Boltzmann constant and T the local (translational) gas temperature. We assume that sufficient accuracy is provided by the approximation

$$\nu(\nu) \approx \nu_0 \phi(\nu_0) \quad (6)$$

We measure species concentrations in moles/cm³ and denote the concentration of a lower (upper) lasing state by n_L (n_U). These concentrations are related to the HF concentrations n_v in the v^{th} vibrational state, and we approximate this relation by

$$n_L = \delta(2J+1) e^{-\delta J(J+1)} n_v, \quad (7)$$

where

$$\delta = \Theta_r/T$$

and, for HF,

$$\Theta_r = 30.16^\circ\text{K}^2 \quad (8)$$

Thus we assume (justifiably) that the populations of the rotational levels are in thermodynamic equilibrium at the translational temperature T . We introduce the rigid rotator approximation for the energy levels as a mathematical simplification which does not alter the calculation of vibrational populations too seriously. Finally, we note that the specific intensity of any steady state lasing mode is not significantly affected by spontaneous emission processes and obtain as our basic transport equation for the specific intensity $I_v(\vec{r}, \vec{\Omega})$ for such a mode

$$(\Omega \cdot \nabla) I_v = h N_A \nu \phi(\nu) B_{LU} \times \left[\left(\frac{2J+1}{2J-1} \right) n_U - n_L \right] I_v, \quad (9)$$

where N_A is Avogadro's number.

We will solve Eq. (9) for the case of slab geometry in which we measure radiation propagation angle $\mu = \cos \theta$ from the z -axis and will assume that for any CW lasing mode we can idealize the appropriate Fabry-Perot mode through the representation

$$I_v = \frac{1}{2\pi} \left(I_v^+(x, z) \delta(\mu-1) + I_v^-(x, z) \delta(\mu+1) \right), \quad (10)$$

where I_v^\pm has the physical significance energy flux per unit area per unit frequency in the $+z$ ($-z$) direction. Because the flow quantities are assumed not to depend on the y -coordinates, the energy fluxes are independent of y also. The further develop-

ment of the lasing theory will employ certain integrals of these energy fluxes as basic variables of the theory.

IV. THRESHOLD GAIN CONDITIONS

The gain in the possible vibrational-rotational transitions depends on the average populations in the molecular levels involved, namely

$$\begin{aligned} \tilde{N}_{v,J}(x, y) = & \frac{1}{L} \int_0^L dz n_v(x, y, z) T^{-3/2}(x, y, z) \\ & \times \exp \{-J(J+1)\Theta_r/T(x, y, z)\} \end{aligned} \quad (11)$$

and, for the total population in the J^{th} rotational level,

$$\begin{aligned} \tilde{N}_{\text{Tot},J}(x, y) = & \frac{1}{L} \int_0^L dz n_{\text{Tot}}(x, y, z) T^{-3/2}(x, y, z) \\ & \times \exp \{-J(J+1)\Theta_r/T(x, y, z)\}, \end{aligned} \quad (12)$$

where

$$n_{\text{Tot}} = \sum_{v=0}^3 n_v. \quad (13)$$

Specifically, it follows from Eqs. (3) - (8) that the zero power gain in the P-branch transition $U \rightarrow L$ is given by

$$\tau_{v,J}(x, y) = S_0 F_{v,J} \left[\tilde{N}_{v+1,J-1} - \tilde{N}_{v,J} \right], \quad (14)$$

where

$$\begin{aligned} S_0 = & \left(\frac{4\sqrt{2}}{3} \pi^{5/2} \times 10^{-38} \right) \left(\frac{\text{MW}}{\text{k}} \right)^{1/2} \left(\frac{N_A \Theta_r L}{h} \right) \\ = & 4.436 \times 10^{11} L \quad \text{for HF} \end{aligned} \quad (15)$$

and

$$F_{v,J} = J(1+0.06J)(v+1). \quad (16)$$

Thus the effective evaluation of \tilde{N} becomes a central problem of the laser.

A first evaluation of the quantities $\tilde{N}_{v,J}$ is readily made, since it is intended that the optics package be implemented after a hydrodynamics and chemistry (without lasing) calculation has been run and, thus, after converged values of $N_v(x, y, z)$ have been obtained. With these populations $\tilde{N}_{v,J}$ may be obtained and $T_{v,J}$ computed for all $v \leq 2$ and $J \leq J_{\max}$. For most purposes it should be adequate and sufficiently inexpensive of computer time to take $J_{\max} = 20$.

The threshold gain G is given here in terms of the mirror reflectivities r_0 at $Z=0$ and r_L at $Z=L$ as

$$G = -\ln(r_0 r_L)^{1/2} \quad (17)$$

although mirror and volume losses could be included, if desired. For each computational cell in the mirror region the quantities $\tau_{v,J}$ are evaluated using zero-power vibrational populations. If

$$\tau_{v,J} < G \text{ for } v \leq 2 \text{ and } J \leq J_{\max} \quad (18)$$

then no lasing occurs in the computational cell, and no explicit changes in the hydrodynamic variables or the chemical populations need be considered. Implicit changes will occur, however, for the lasing in other portions of the gas will alter the gas temperature with effects on both the hydrodynamics and the chemistry.

If the inequality of Eq. (18) is violated, then lasing occurs in the computational cell. It is assumed to occur on all the permitted vibrational transitions at the P-branch rotational quantum number J^* defined from the zero-power gains by the conditions

$$\tau_{1,J^*} = \max_{1 \leq J \leq J_{\max}} \tau_{1,J} \quad (19)$$

Then the CW lasing condition is imposed through the relations

$$\tau_{v,J^*} = G, \quad \text{for } 0 \leq v \leq 2 \quad (20)$$

This provides a set of integral constraints on the vibrational populations.

It is possible to approximate and simplify the set of integral constraints of Eq. (20) by noting that the difference of the exponential in the integrand of \tilde{N}_{v,J^*-1} and \tilde{N}_{v,J^*} , namely

$$\exp[-2J^* \theta_r / T] \quad ,$$

does not greatly affect the value and integral of Eq. (11). If $T_0(x)$ denotes the maximum value of the gas temperature profile, then the above factor may with sufficient accuracy be replaced by

$$B = \exp[-2J^* \theta_r / T_0(x)] \quad (21)$$

Such a replacement is obviously adequate when the temperature profile is flat. When it is sharply peaked the exponential factor may vary significantly with z but then the other exponential factor cuts off the integral much more drastically. We have checked these conclusions with data from RICE calculations⁷ and anticipate that the approximation specified by Eq. (21) will introduce less than a 10% error into the integral of Eq. (11) under essentially all conditions of interest.

It is convenient to introduce the quantities

$$N_v(x, y) = \frac{1}{L} \int_0^L dz n_v(x, y, z) T^{-3/2}(x, y, z) \times \exp[-J^*(J^*-1)\theta_r / T(x, y, z)] \quad (22)$$

$$N_{\text{Tot}}(x, y) = \sum_{v=0}^2 N_v(x, y) \quad (23)$$

and

$$N_{\text{Tot}}(x, y) = \frac{1}{L} \int_0^L Jz n_{\text{Tot}}(x, y, z) \quad (24)$$

Of course, when the flow geometry is composed of N equal reaction zones of width h , i.e. $L = Nh$, only one of these zones is usually computed and the averaging operator $\bar{}$ may be replaced by an average

over h , i.e.

$$0 = \frac{1}{L} \int_0^L dz = \frac{1}{h} \int_0^L dz \quad (25)$$

Normally the quantities specified by Eqs. (22) - (24) will be assumed independent of y . Then the gain conditions of Eq. (20) may be restated as

$$G = \sum_0 F_{v,J^*} \left[N_{v+1} - BN_v \right] \quad \text{for } v=0, 1, 2, \quad (26)$$

a set of equations which specify N_v in terms of T , N_{Tot} , G , L and J^* .

V. INTEGRAL CONSTRAINTS ON THE VIBRATIONAL POPULATIONS

The constraints provided by Eq. (26) may be converted to explicit solution for N_v in terms of N_{Tot} , B and the quantities

$$H_v = \frac{G}{\sum_0 F_{v,J^*}} \quad \text{for } v=0, 1, 2 \quad (27)$$

Solution of the set of linear equations for N_v yields

$$N_0(x, y) = \left(1 - B^4\right)^{-1} \left[(1-B)N_{\text{Tot}}(x, y) - (1-B^3)H_0 - (1-B^2)H_1 - (1-B)H_2 \right], \quad (28)$$

$$N_1 = \left(1 - B^4\right)^{-1} \left[B(1-B)N_{\text{Tot}} + (1-B)H_0 - B(1-B^2)H_1 - B(1-B)H_2 \right], \quad (29)$$

$$N_2 = \left(1 - B^4\right)^{-1} \left[B^2(1-B)N_{\text{Tot}} + B(1-B)H_0 + (1-B^2)H_1 - B^2(1-B)H_2 \right], \quad (30)$$

and

$$N_3 = \left(1 - B^4\right)^{-1} \left[B^3(1-B)N_{\text{Tot}} + B^2(1-B)H_0 \right]$$

$$+ B(1-B^2)H_1 + (1-B^3)H_2 \quad (31)$$

Thus when values for n_{Tot} and T are available, the integral constraints (N_v) on the vibrational populations are provided by Eqs. (28) - (31) for any lasing region of the gas.

However, additional integrals over the vibrational populations are required to specify the average intensity of radiation in the lasing cavity. For this purpose we suggest an approximation to the correct vibrational distribution in the gas which is consistent with Eqs. (28) - (31), correct in the limit of no z variations in the system and not inconsistent with the (known) distribution of $n_{\text{Tot}}(x, y, z)$. Specifically, we define

$$H_v(x, y, z) = \frac{1}{N} T^{3/2}(x, y, z) \exp \left[-J^*(J^*-1)\theta_r/T(x, y, z) \right] H_v \quad \text{for } v=0, 1, 2 \quad (32)$$

and propose for the vibrational distributions

$$n_0(x, y, z) = \left(1 - B^4\right)^{-1} \left[(1-B) - (1-B^3)H_0(x, y, z) - (1-B^2)H_1(x, y, z) - (1-B)H_2(x, y, z) \right] n_{\text{Tot}}(x, y, z) \quad (33)$$

and in more compact notation,

$$n_1 = \left(1 - B^4\right)^{-1} \left[B(1-B) + (1-B)H_0 - B(1-B^2)H_1 - B(1-B)H_2 \right] n_{\text{Tot}} \quad (34)$$

$$n_2 = \left(1 - B^4\right)^{-1} \left[B^2(1-B) + B(1-B)H_0 + (1-B^2)H_1 - B^2(1-B)H_2 \right] n_{\text{Tot}} \quad (35)$$

and

$$n_3 = (1-B^4)^{-1} \left[B^3(1-B) + B^2(1-B)H_0 + B(1-B^2)H_1 + (1-B^3)H_2 \right] n_{Tot} \quad (36)$$

We anticipate that Eqs. (33) - (36) could be used in self-consistent calculations of the flow field, the gas temperature, the radiation field and the chemical concentrations until the calculation has largely converged. Only as a last refinement would it be necessary to turn to the rate equations for n_v for an "exact" solution and, since n_v is not used explicitly in calculations of the hydrodynamic variables and the radiation field, such "exact" solutions would serve primarily to check the convergence of the calculation. The convergence properties of the theory are essentially unexamined, but it is presumably permissible to introduce exact rate equations for n_v at any convenient stage of the iteration process.

VI. AVERAGE INTENSITY OF RADIATION

For each of the lower vibrational states $v=0, 1, 2$ we define a line integrated specific intensity by

$$I_v^\pm(\vec{r}) = \int_{\text{emission line}} d\nu I_v^\pm(\vec{r}) \quad (37)$$

The range of frequency integration is different in each case because of the differing vibrational constants of the lasing levels. Because the gain in the system is small, an adequate description of the specific intensity is provided by the average total density.

$$I_v(x, y) \equiv \frac{1}{L} \int_0^L dz \left[I_v^+(\vec{r}) + I_v^-(\vec{r}) \right] \quad (38)$$

In particular, the power emitted per unit area in the xy plane, P , is determined by

$$P(x, y) = G [I_0(x, y) + I_1(x, y) + I_2(x, y)] \quad (39)$$

and the total power emitted is

$$P = \int_0^L dy \int_{x_0}^{x_0+d} dx P \frac{erg}{sec} \quad (40)$$

The chemistry equations for the vibrational populations are used to provide values of I_v .

VII. RADIATIVE CORRECTIONS TO HYDRODYNAMICS AND CHEMISTRY EQUATIONS

The direct effect of the volume emission of photons on the hydrodynamics of the system is a radiative correction to the time rate of change of specific total energy E . This correction may with sufficient accuracy be expressed in terms of the quantities I_v and the defined quantities

$$F_v = F_v, J^* T^{-3/2}(x, y, z) \exp \left[-J^*(J^*-1) \Theta_I/T(x, y, z) \right] \quad (41)$$

and

$$g_v = \frac{1}{L} s_0 F_v \left[n_{v+1} - B n_v \right]$$

as

$$\left[\frac{D}{Dt} \rho E \right]_{\text{rad}} = - (g_0 I_0 + g_1 I_1 + g_2 I_2) \quad (42)$$

The approximate treatment of the temperature profile in Eq. (42) is consistent with the approximation introduced in the treatment of the integral constraints. The rapid variations in z of the density and temperature factors justify the use of I_v . The direct effect is, of course, a decrease in temperature in the lasing region. This affects the hydrodynamic motion by changing the pressure distribution in the gas and affects the chemical reactions in the system by changing the reaction rates.

The chemistry equations for species other than HF and for $n_{Tot}(x, y, z)$ are otherwise unchanged by the presence of lasing. The additional equations needed to complete the description of the chemical reactions may be written symbolically as

$$\frac{D}{Dt} n_v = \nabla \cdot (D \nabla n_v) + \left[\frac{D}{Dt} n_v \right]_{\text{chem}}$$

$$+ \frac{1}{N_A h \nu_0} (g_v I_v - g_{v-1} I_{v-1}), \quad (43)$$

with the convention that

$$I_{-1} = 0. \quad (43a)$$

The chemical reaction terms may be treated with any desired level of completeness, but will typically include a creation term, giving a population distribution over the vibrational states due to the reaction $H_2 + F \rightarrow HF^* + H$, and vibrational de-excitation terms. As an example, we display a set of reaction terms that might suffice for an approximate description of some lasing systems. The reactions and the notation are taken from a report by Cohen.⁸ Thus

$$\left[\frac{D}{Dt} n_0 \right]_{\text{chem}} = k_{4a} n_F n_{H_2} + k_{6a_1} n_{\text{Tot}} n_1 + k_{6b_1} n_F n_1 + k_{6g_1} n_{H_2} n_1, \quad (44)$$

$$\left[\frac{D}{Dt} n_1 \right]_{\text{chem}} = k_{4b} n_F n_{H_2} + (k_{6a_2} n_2 - k_{6a_1} n_1) n_{\text{Tot}} + (k_{6b_2} n_2 - k_{6b_1} n_1) n_F + (k_{6g_2} n_2 - k_{6g_1} n_1) n_{H_2}, \quad (44a)$$

and

$$\left[\frac{D}{Dt} n_2 \right]_{\text{chem}} = k_{4c} n_F n_{H_2} + (k_{6a_3} n_3 - k_{6a_2} n_2) n_{\text{Tot}} + (k_{6b_3} n_3 - k_{6b_2} n_2) n_F + (k_{6g_3} n_3 - k_{6g_2} n_2) n_{H_2}. \quad (44b)$$

We emphasize, however, that the theory is developed without specific limitation on the chemical reactions adopted for the system.

VIII. EVALUATION OF THE TOTAL INTENSITIES AND THE HF CONCENTRATIONS

We recall that no species diffusion occurs through the walls at $z=0, L$. Thus a correct boundary condition at these walls is

$$\frac{\partial}{\partial z} n_v = 0 \quad \text{at } z = 0, L. \quad (45)$$

A set of equations for I_v may be obtained by averaging Eq. (43) over the z -direction. Define for any quantity $Q(z)$ the average by

$$\langle Q \rangle \equiv 0Q \equiv \frac{1}{L} \int_0^L dz Q(z). \quad (46)$$

Then we obtain from Eqs. (43) and (26)

$$\frac{G}{N_A L h \nu_0} (I_v - I_{v-1}) = \left\langle \frac{D}{Dt} n_v \right\rangle - \frac{\partial}{\partial x} D \frac{\partial}{\partial x} \langle n_v \rangle - \left\langle \left[\frac{D}{Dt} n_v \right]_{\text{chem}} \right\rangle. \quad (47)$$

Solving for I_v yields

$$I_v = \left(\frac{N_A L h \nu_0}{G} \right) \sum_{j=0}^v \left(\left\langle \frac{D}{Dt} n_v \right\rangle - \frac{\partial}{\partial x} D \frac{\partial}{\partial x} \langle n_v \rangle - \left\langle \left[\frac{D}{Dt} n_v \right]_{\text{chem}} \right\rangle \right). \quad (48)$$

The quantities I_v may be eliminated from Eq. (43) using Eq. (48). The result is a set of coupled partial integro-differential equations for the species concentrations. These equations would normally be solved iteratively and several iterative procedures seem natural for the problem. It is not presently known how much flexibility there is in the choice of acceptable iterative procedure. Here we simply put forward one procedure which is consistent with the iterative procedures adopted in the RICE code.¹ The procedure was proposed by the RICE investigators.⁷

We presume the iterations are started after converged values for hydrodynamic variables and for species concentrations are available from numerical evaluation of the theory without lasing. From these variables one may complete a first iterative step to obtain values n_v^1 for the vibrational populations and values I_v^1 for the total intensity by successive substitutions into Eqs. (33) - (36) and (48). The values of n_v^1 obtained from Eqs. (33) - (36) should be used in Eq. (48) to obtain I_v^1 .

The iterative process may be continued by using the first iteration to provide evaluations of the radiative terms in the internal energy equations and the vibrational population equations. Specifically, we propose that the internal energy term be approximated by

$$\left[\frac{D}{Dt} (\rho E)^1 \right]_{\text{rad}} = - \sum g_v^1 I_v^1, \quad (49)$$

where

$$g_v^1 = \frac{1}{L} s_o F_v \left[n_{v+1}^1 - B n_v^1 \right], \quad (50)$$

and the contribution to Eq. (43) be approximated by

$$\left[\frac{D}{Dt} n_v^1 \right]_{\text{rad}} = \frac{1}{N_A h \nu_o} \left[g_v^1 I_v^1 - g_{v-1}^1 I_{v-1}^1 \right]. \quad (51)$$

These terms would be used to correct values of the corresponding variables, as done in the other parts of the RICE program, by integrating one time step using the radiative term as the source for the time rate of change, e.g.

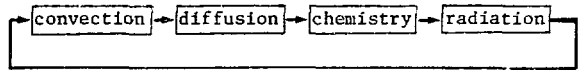
$$\frac{\partial}{\partial t} n_v = \left[\frac{D}{Dt} n_v^1 \right]_{\text{rad}}, \quad (52)$$

and, for later stages of the iterations, when n_v^n has been determined and the $(n+1)^{\text{st}}$ cycle has been completed through the chemical reactions and the determination of the new radiation intensities I_v^{n+1} , the radiative changes in n_v , yielding n_v^{n+1} will be determined from

$$\frac{\partial}{\partial t} n_v = \left[\frac{D}{Dt} (n_v^{n+1}) \right]_{\text{chem}} - \left[\frac{D}{Dt} n_v^n \right]_{\text{rad}}. \quad (53)$$

We presume that Eqs. (52) and (53) would be discretized by either totally explicit or totally implicit differencing to preserve the value of n_{Tot} at each point. The requirement that N_v be conserved is more awkward to meet. The obvious way to conserve N_v , the addition of a term λn_v^1 to the algebraic expression for n_v^2 with λ chosen to satisfy conservation, violates local conservation of n_{Tot} . We think that the best procedure would be to add the λn_v^1 term for $v=0, 1, 2$ and then determine n_3^2 from n_{Tot} . The requirement for N_3 is then satisfied automatically, and the possible difficulty of the procedure, negative values for $n_v(z)$ for some range of z , will hopefully disappear as converged values of n_v are reached.

Iterations would proceed by adding one link, the radiative stage, to the RICE chain of iteration



displayed above. In each link of the cycle the hydrodynamic variables and species concentrations calculated in the previous link are used to evaluate the source terms in the link under consideration. One ambiguity in this prescription is in the treatment of the vibrational populations in the radiative link. It is presently imagined that n_v evaluated in the chemistry link would be used in Eq. (48) to obtain I_v . The same n_v and I_v would be used to evaluate the radiative source terms of Eqs. (42) and (43). However, it is certainly possible that convergence would be speeded by inserting a computation of new vibration populations n_v from Eqs. (33) - (36) before computing new values of I_v in the early iterative loops and omitting this step only after the temperature distribution has largely converged. We do not presently know which procedure would be more efficient.

IX. POSSIBLE MODIFICATIONS TO THE RICE CALCULATION-AL SCHEME

We would anticipate that the discrete changes in $\partial n_v / \partial x$ and I_v that occur when threshold conditions for lasing are met, when J shifting occurs, and when cut-off occurs will cause appreciable inaccuracies in the RICE computation unless special precautions are taken to subdivide the computational cell where such a discrete change occurs. Certainly, previously reported calculational methods,^{2,4,6} which were essentially an integration in the x-coordinate only, have required the determination of the value of x_c at which such a discontinuity occurred and the stipulation that such an x_c be an edge of a computational cell. The location of x_c will change during the course of the iteration, so it is necessary to determine x_c self-consistently during the calculation. One procedure for accomplishing this is discussed by Emanuel.⁴

It is also possible that in some configurations the threshold condition for lasing is met at $x_{\text{threshold}} < x_0$. Under these conditions results with the RESALE program⁴ have been that it is necessary to modify the discontinuous change in mirror reflectivities at x_0 postulated in the present model in order to obtain computational results. This might be an artifact of the one-dimensional x-integration being used in the model. If, on the other hand, large resolved spatial variations cause difficulties to time dependent calculations, we would expect the RICE program to exhibit similar phenomena. If it does, the RESALE program⁴ again provides a possible model for this feature.

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