Note

Numerical Procedure for a Pulsed DF–CO$_2$ Transfer Laser*

I. INTRODUCTION

Recently, a numerical procedure for constant-gain chemical laser calculations was presented which accounted for J-shifting of the laser transition [1]. It was postulated that, at any particular time during lasing, only a single transition (corresponding to a particular rotational quantum number J) between any two adjacent vibrational levels is involved in lasing. Other transitions, involving other rotational states, correspond to smaller gain coefficients and therefore do not satisfy the lasing threshold conditions [2]. This conjecture resulted from the assumption that the rotational populations for a given vibrational level are in a Boltzmann distribution at the translational temperature (valid if the characteristic time to achieve the distribution is short compared to the stimulated emission time).

In practice, however, this single, J-shifting transition mode of operation does not prevail. Spectral measurements on a high-pressure, pulsed DF-CO$_2$ transfer laser showed that the strongest lines were generally either $P(18)$ or $P(20)$, with most of the laser energy concentrated in two or three P-branch transitions centered on these lines [3]. Calculations indicated that the rotational–translational equilibration time was much shorter than the stimulated emission time in these experiments, so the rotational populations of the lasing vibrational levels should have been in a Boltzmann distribution at the translational temperature. Thus, although the criterion given for single-line lasing [2] was met in these experiments, lasing was observed on several lines with the dominant transitions remaining around $P(18)$ and $P(20)$ for the entire pulse. Furthermore, any tendency for lasing to shift to the rotational transition corresponding to maximum gain could be negated by the fact that the laser cavity is tuned with a conventional electric-discharge laser having a dominant transition at $P(20)$. Since the laser cavity is not retuned during the pulse emission, the shift of maximum gain toward different J-values during the pulse is not manifested with respect to the spectra of laser output. Thus a provision for J-shifting in any computational model is probably not justified.

In addition to the results of [1] the idea of using a single rotational transition in simplified calculations has been explored. For example, approximate closed-form

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expressions for the intensity, energy, and chemical efficiency of an $F + H_2$ laser oscillator were obtained in [4] by assuming a constant translational-rotational temperature, considering only predominant reactions (assumed to be uni-directional in their dominant direction) and restricting application to a Doppler-broadened gain profile. For the situations where these assumptions are valid, these expressions are in good agreement with the results of the more complicated numerical procedure in [1].

Another recent paper [5] presents simple expressions for the intensity, energy, and efficiency of the pulsed $DF-CO_2$ chemical transfer laser, but these relations were derived with the restriction that the level of initiating radicals was low. Generally, this assumption would restrict the applicability of this method to pulses of long duration (reduced peak intensity). For the low levels of initiation for which this method was valid, it gave excellent agreement with the more comprehensive model [1] and experiment.

The purpose of this communication is to present a procedure, which is inter-mediate in simplicity between the more complicated method [1] and the highly simplified schemes [4, 5], for calculating the pulse profile and the intracavity conditions of a pulsed $DF-CO_2$ laser. The primary assumptions of the associated theoretical model are:

(1)   The radiation field in the cavity will begin oscillating in a quasisteady-state when the gain reaches threshold. Thereafter the gain will remain at threshold until the pulse terminates. The neglect of transient oscillation phenomena in the cavity radiation field is valid since the important molecular processes occurring in the laser medium have characteristic times at least two orders of magnitude longer than the mean photon lifetime in the oscillator [6].

(2)   The correct shape of the laser transition line (Lorentzian with Doppler corrections is appropriate for high pressure lasers) is utilized rather than using the Doppler-broadened line as an approximation. We are able to avoid this approxi-mation since complicating derivatives [1] are unnecessary in the present numerical procedure.

(3)   For reasons discussed above, J-shifting is neglected in this model, and the $P(20)$ transition is assumed to be dominant for the duration of the pulse. For computational purposes, only a single line, corresponding to the dominant transition, is used.

Thus, the present model includes all of the physical features of the earlier complex model [1] with the exception that J-shifting is neglected. In addition, for the case of high-pressure transfer lasers, a more realistic laser transition line can be utilized since a Lorentzian or Voight profile does not lead to mathematical intractability in the present procedure.

II. EQUATIONS

In the DF–CO$_2$ transfer laser, different energy modes or groups of modes can be treated as single reservoirs of energy due to the quasiequilibrium existing among the various levels in those modes [3]. For the present model the various energy modes are grouped as follows:

Group 1—rotational and translational energy modes;

Group 2—symmetric–stretching and bending modes of CO$_2$;

Group 3—asymmetric–stretching mode of CO$_2$;

Group 4—vibrational mode of DF.

The quasi-thermodynamic approach taken by Gordietz [7] is utilized and Maxwell–Boltzmann distributions (or Treanor distributions when the need arises [8]) are assumed for the energy level populations in each group of energy modes.

With the various energy modes lumped into Groups 1 through 4 and the assumption of the quasisteady state for the radiation field, the pulse chemical laser can now be represented by $13 + N$ first order, nonlinear differential equations of the type

$$dQ_i/dt = S_i + \epsilon_i \alpha I. \tag{1}$$

In this model Q_1 to Q_4 refer to the respective energy densities of Group 1 to 4, and Q_i, $i > 4$, refer to the various chemical species. The symbol S_i denotes the production rate of the ith energy group or species by chemical, collisional energy-exchange, and spontaneous radiative processes. The term $\epsilon_i \alpha I$, where α and I are the gain and radiation intensity, respectively, represents stimulated radiation. Thus, $\epsilon_1 = 0$, $\epsilon_2 = \nu_1/\nu$, $\epsilon_3 = -\nu_3/\nu$, and, for $i > 3$, $\epsilon_i = 0$, where $h\nu_1$ and $h\nu_2$ are the energies for the lower and upper laser levels, respectively, and $h\nu$ is the photon energy of the stimulated radiative process

The required initial conditions (i.e., the values of Q_i at $t = 0$) are obtainable from the controllable parameters being studied such as initial pressure, temperature, reactant ratios, cavity dimensions, and initial radical concentration (for ignition). Because of the quasithermodynamic treatment of energy, initial energy densities of Groups 1–4 can be obtained easily from the initial temperature and pressure. Initial concentrations of reactants can be obtained from initial temperature, pressure, and reactant ratios.

For steady-state oscillations in the laser cavity, the gain coefficient α can be approximated [9] as

$$\alpha_{\text{th}} = -(\tfrac{1}{2} \ln r)/L, \tag{2}$$

where r is the reflectivity of the laser output mirror and L is the cavity length. The subscript on α_{th} denotes it as the "threshold" gain. The gain coefficient is also expressible [3] in terms of the variables Q_1, Q_2, Q_3, and Q_6, where Q_6 is the molar concentration of CO_2; thus we have the constraint

$$\alpha_{th} = f(Q_1, Q_2, Q_3, Q_6). \tag{3}$$

III. NUMERICAL PROCEDURE

A numerical integration scheme was formulated to solve the system of equations represented by Eqs. (1)–(3). Since the radiation intensity I is an undetermined function of time, it was obtained at each time increment of integration by iteration. A modification of Hamming's predictor-corrector method [10] for nonlinear differential equations provided the most direct means for accomplishing this task.

The iterative procedure used to obtain the radiation intensity function $I(t)$ at each increment of integration with respect to t is as follows: (a) The gain expression for steady state oscillation, Eq. (2), is used in Eq. (1). (b) Assuming that all desired quantities $Q_i(t)$ are known at time t, one can march forward to time $(t + \Delta t)$ by using an estimated value for $I(t, t + \Delta t)$, the average value of I between times t and $t + \Delta t$, in Eq. (1). (c) At the end of the integration step, the computed values of the dependent variables $Q_1(t + \Delta t)$, $Q_2(t + \Delta t)$, and $Q_3(t + \Delta t)$ can be used to calculate the gain coefficient by Eq. (3). (d) If the gain $\alpha(t + \Delta t)$ computed by Eq. (3) does not equal the value given by Eq. (2), the "threshold gain," within a tolerance of 0.05%, the integration step is repeated using a second estimate of $I(t, t + \Delta t)$. (e) This second estimate is made via a linear type relationship relating $I(t, t + \Delta t)$ to $\alpha(t + \Delta t)$, much in the same manner as the method of false positions. If the first guess for $I(t, t + \Delta t)$ is $I_1(t, t + \Delta t)$ and yields a gain coefficient α_1 at $t + \Delta t$ that differs from the threshold gain α_{th} by an amount greater than the tolerance, then a second estimate, $I_2(t, t + \Delta t)$, of $I(t, t + \Delta t)$ is made according to

$$I_2(t, t + \Delta t) = G \times I_1(t, t + \Delta t), \tag{4}$$

where $G = 1.05$ if $\alpha_1 > \alpha_{th}$ and $G = 0.95$ if $\alpha_1 < \alpha_{th}$. If the corresponding gain coefficient at $t + \Delta t$, α_2, does not come within the tolerance of α_{th}, then the third estimate of $I(t, t + \Delta t)$, or $I_3(t, t + \Delta t)$ is made according to the linear relation

$$I_3 = I_1 + \frac{I_2 - I_1}{\alpha_1 - \alpha_2} [\alpha_1 - \alpha_{th}]. \tag{5}$$

The foregoing step is iterated, using Eq. (5) to obtain new estimates of $I(t, t + \Delta t)$, I_n, until α_n comes within the tolerance of α_{th}. Generally, once the onset of the

power pulse (gain-switching) occurred, only one or two iterations were necessary to obtain values of α within the tolerance of α_{th}. In fact, the overall computation time for power output of a pulsed laser seldom exceeded that required for the more straightforward small-signal-gain calculation by more than 30 percent.

The iteration procedure was simply placed inside a general Hamming predictor-corrector method subroutine (Fortran IV), and served as a control on whether the next integration step was performed or not.

IV. COMPARISON WITH MORE COMPLICATED SCHEME

In Fig. 1 a power output profile for the pulsed DF–CO₂ transfer laser is given as computed by the scheme outlined above. Also shown (see circles) is the result of a calculation [11] performed by a more complicated scheme [1]. The initial conditions
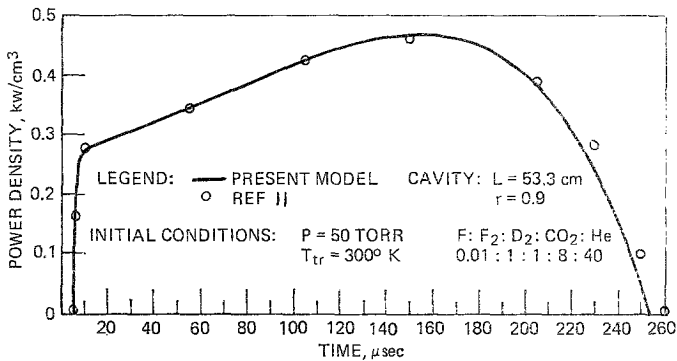

FIG. 1. Power pulse for DF–CO₂ chemical transfer laser.

and rate constants used in the present calculation were the same as those used in the more complicated effort [11]. For convenience, the initial conditions are given in the legend of Fig. 1. As indicated, the agreement between the simple iteration method and the more complicated method is excellent. Integrated pulse energy, peak power output, time of peak power output, and pulse duration obtained by the simple method were 1.70 j/liter, 8.83 kwatt/liter, 150 μsec, and 248 μsec, respectively. The corresponding values obtained by the more complicated method were 1.71 j/liter, 8.64 kwatt/liter, 145 μsec and 255 μsec, respectively.

Time required for the computation of a single laser pulse profile via the simple method presented here was 18 seconds on an IBM 360-91 at the APL computer center.

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J. C. PIRKLE, J.R.

School of Medicine,
The Johns Hopkins University
Baltimore, Md.

T. O. POEHLER AUD V. G. SIGILLITO

Applied Physics Laboratory,
The Johns Hopkins University,
Silver Spring, Md. 20910