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Efficient Model for HF Lasers with Rotational Nonequilibrium

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A method for modeling rotational nonequilibrium in HF(DF) laser systems that significantly reduces the computation time required for such calculations is described. With this formulation, an approximation can be obtained of the nonequilibirum optical gains of the individual v, J transitions without computing the individual populations for each v, J state, which appreciably reduces the number of integration variables. The predictions of a pulsed H_2-F_2 laser model utilizing this approach are very similar to the predictions

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of a more complex model. The computational economy gained makes feasible parametric studies to improve understanding of the importance of rotational relaxation in laser calculations.

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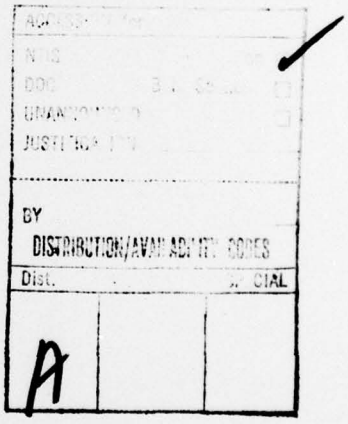

EFFICIENT MODEL FOR HF LASERS WITH ROTATIONAL NONEQUILIBRIUM

Rotational relaxation and rotational hole-burning play an important role in determining the degree of saturation and the rate at which energy can be extracted from a chemical-laser medium. Model predictions of laser output energy, spectral content, and performance under line-selected operation are more realistic when rotational-relaxation mechanisms are included. Mode structure and mode competition within an optical cavity are directly related to the distribution of gain and losses within the cavity. Laser-output beam-quality predictions should be made with a model that can accurately predict the gain distribution within the active medium. Satisfactory prediction of gain distribution requires that the effects of rotational nonequilibrium be considered.

Rotational relaxation has been modeled either by means of detailed rotational kinetics[1-6] or by use of a rotational relaxation time constant.[6,7] The detailed kinetics model is more realistic, and appears to have the potential of being able to predict time histories of the laser transitions in all the comprehensive detail that is seen in experiments. In contrast, a time constant model seems to display the dominant features of this time-resolved spectra while missing some fine details. Preliminary comparisons of laser output energy and spectral energy distributions, however, have not shown substantial differences in the two modeling approaches.[6] More exhaustive comparisons between the models and with experimental spectra need to be

carried out in order to identify regimes where the additional realism afforded by the detailed kinetics model will be required.

A difficulty with HF laser models treating finite rate rotational relaxation is their need for large amounts of computation time. The method described here increases the efficiency of models in which the time-constant approach is used. This new scheme drastically reduces the computational time, with little loss of accuracy. In a comparison with a comprehensive earlier model (ROLAX)[6] for chain-reaction HF lasers, the number of integration variables can be reduced from 179 to 65, and computation times are typically shorter by a factor of 10 or more. For the two models, predictions of pulse energy, pulse length, and spectral energy distribution typically agree within 5%.

Formulation of the new model through our Eq. (4) is identical to that given in Ref. 7. This material is recapitulated very briefly. The major assumptions are: (1) Kinetic processes are represented by 164 reactions, based on the survey by Cohen.[8] (2) The reacting mixture is homogeneous and contained in a Fabry-Perot laser cavity. (3) Lasing is assumed to be always in the P-branch and restricted to the first fifteen transitions in each of the lowest six vibrational bands. (4) All transitions are assumed to have low initial intensities, which grow if the gains rise above threshold.

HF vibration-rotation state populations N(v, J) are computed from the kinetic reactions, with the effects of lasing, absorption, and spontaneous emission taken into account.

The gain coefficient is

$$\alpha(v,J) = \frac{hN_A}{4\pi}\,\omega_c(v,J)\,\varphi_c\,B(v,J)\left[\frac{g_\ell}{g_u}\,N(v+1,\,J-1) - N(v,J)\right] \qquad (1)$$

where v and J are quantum numbers of the lower level of the transition, $\omega_c(v,J)$ is the wavenumber of the transition, $B(v,J)$ is an Einstein coefficient, g_u and g_ℓ are upper and lower state degeneracies, respectively, and $N(v,J)$ are state populations. Both Doppler and pressure broadening are considered through use of a Voigt profile φ_c, which is evaluated at line center.

The rate of photon extraction per unit volume is

$$\chi_{rad}(v,J) = \alpha(v,J)\,f(v,J) \qquad (2)$$

where $f(v,J)$ is photon flux. The rate equation for f is

$$\frac{df(v,J)}{dt} = c\left(\frac{L}{\ell}\right)\left[\alpha(v,J) - \alpha_{th}\right] f(v,J) \qquad (3)$$

where c is the speed of light and

$$\alpha_{th} = -\frac{1}{2L}\ln\left(R_O R_L\right) \qquad (4)$$

where L is the length of the active medium, ℓ is the mirror spacing, and R_O and R_L are mirror reflectivities.

For brevity and clarity, the new rotational relaxation model is explained in terms of a single vibrational band laser. A discussion of the formulation for a multiband laser with cascading will be given elsewhere because of its length. Numerical results given here, however, are for the full multiband model.

Let $N_u(J)$ and $N_\ell(J')$ denote the upper and lower state populations, respectively, of a laser transition with photon flux f. The rate equations for the populations may be written

$$\frac{dN_u(J)}{dt} = -\alpha f + \frac{N_u^e(J) - N_u(J)}{\tau_u(J)} \tag{5a}$$

and

$$\frac{dN_\ell(J')}{dt} = \alpha f + \frac{N_\ell^e(J') - N_\ell(J')}{\tau_\ell(J')} \tag{5b}$$

where $N_i^e(J)$ is the instantaneous rotationally equilibrated concentration of $N_i(J)$ and $\tau_i(J)$ is the time constant for rotational relaxation of level $N_i(J)$.

The rotational relaxation mechanism represented by Eq. (5) is identical to the formulation used in Ref. 7, except that preferential (i.e., J-selective) pumping and deactivation are ignored. Here, individual rotational states are fed (or depleted) only through rotational relaxation or lasing. Pumping and vibrational-state deactivation are manifested indirectly through their effect on N^e terms.

The relaxation time τ is assumed to depend on the energy separation of adjacent rotational states. The form[7]

$$\tau_J \sim A_J \exp\left(\frac{B\Delta E_J}{kT}\right) \tag{6}$$

is used, where A_J^{-1} is proportional to the frequency for binary collisions with all partners, B is a constant, and ΔE_J is the energy separation of adjacent rotational states.

For P-branch transitions a useful approximation is

$$\tau_u \cong \tau_\ell \equiv \tau \tag{7}$$

For this single-band system, Eq. (1) may be written

$$\alpha(J) = \phi\left[\frac{g_\ell}{g_u} N_u(J) - N_\ell(J')\right] \tag{8}$$

where ϕ_J represents all quantities outside the brackets in Eq. (1). A rotationally equilibrated gain α^e is defined as

$$\alpha^e(J) = \phi\left[\frac{g_\ell}{g_u} N_u^e(J) - N_\ell^e(J')\right] \tag{9}$$

Differentiating Eq. (8) with respect to time, and substituting Eqs. (5) and (7) through (9), one obtains

$$\frac{d\alpha}{dt} = -\phi\left(\frac{g_\ell}{g_u} + 1\right)\alpha f + \frac{\alpha^e - \alpha}{\tau} \tag{10}$$

At saturation, $\alpha \cong \alpha_{th}$ = constant. Therefore, $d\alpha/dt = 0$ and Eq. (10) can be solved for α to obtain

$$\alpha = \frac{\alpha^e}{1 + f/f_s} \tag{11}$$

where the "saturation flux" f_s is defined by

$$f_s \equiv \frac{1}{\phi\left[(g_\ell / g_u) + 1\right]\tau} \tag{12}$$

Although Eq. (11) was derived with the use of the saturation assumption, it is clearly valid for the case $f \ll f_s$ since it reduces to $\alpha \cong \alpha^e$. The calculations in Ref. 7 from a rotational equilibrium model ($\alpha = \alpha^e$) indicate that the saturation process is rapid enough such that, prior to saturation, the condition $f \ll f_s$ generally holds. Thus, Eq. (11) may be taken to apply at all times with very little error. This result makes it possible to predict the nonequilibrium gains of the individual vibrational-rotational transitions directly from the vibrational populations and the photon fluxes of the corresponding transitions. The need to compute instantaneous rotational state populations is avoided, thus eliminating them as required integration variables.

A rotational bottle-necking effect is clearly demonstrated by Eq. (11). The observed laser intensity depends on the magnitude of the saturation intensity f_s, i.e., for small f_s, f must remain small. Since f_s is

proportional to $1/\tau$, the rate at which energy is pumped into (or extracted from) the laser inversion is limited by rotational relaxation.

From Eq. (6), τ_J increases with increasing J. Therefore, f_s is a decreasing function of the rotational quantum number. Rotational bottlenecking becomes stronger as J increases. At the same time, because of the increased rotational energy spacings, collisional quenching is believed to be less rapid with increasing J. An energy trapping-like characteristic results, which may be a contributing factor in the comparatively long but low-powered laser emissions observed for high J transitions.*

The preceding formulation was extended to a multilevel system, and its predictions compared with those of the comprehensive rotational nonequilibrium model of Ref. 6. The major distinction between the two models is in the calculation of gain. The model described in Ref. 6 keeps track of the population of each v, J state and uses these in Eq. (1) to determine the gain for each transition. The present model keeps track of only the vibrational state populations. The Boltzmann distribution then is applied to obtain the equilibrated gains α^e, which are subsequently utilized in the multiband counterpart of Eq. (11) to obtain the nonequilibrium transition gains. The kinetics utilized in both models are identical. For consistency, the relaxation time-constant version of the Ref. 6 model is used.

A comparison of the predicted pulse outputs of the two models for an atmospheric pressure H_2-F_2 laser is given in Fig. 1. The pulses are nearly identical, even to the details of the individual "bumps" in the pulse shapes.

*J. S. Whittier and R. Hofland, private communication, The Aerospace Corporation, El Segundo, California.

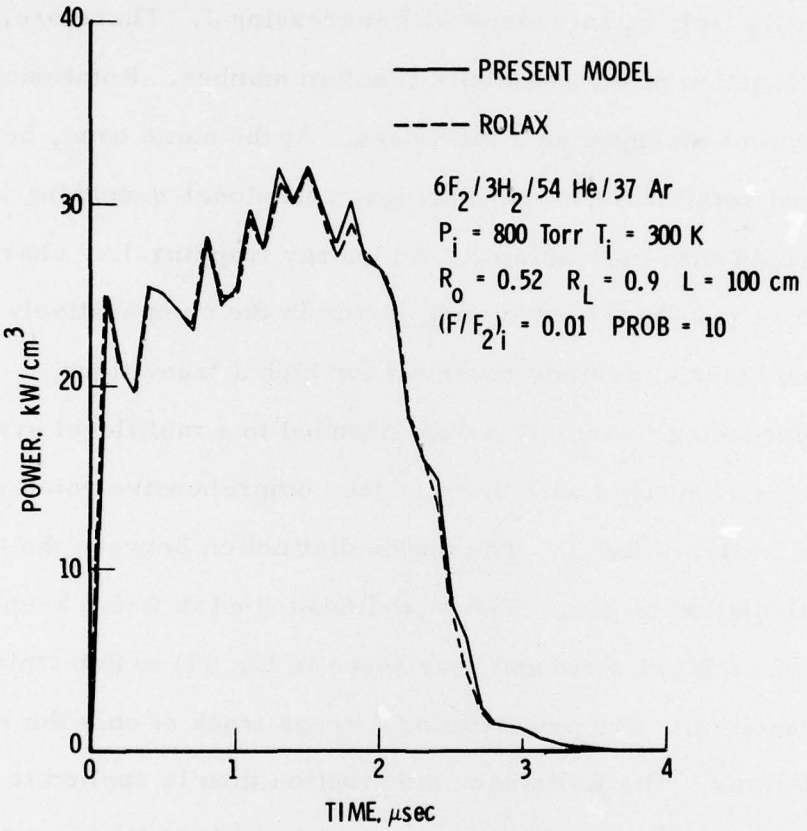

Fig. 1. Comparison of Pulse Outputs Predicted by Present Model and ROLAX

In Fig. 2, the model predictions of time resolved spectra for the same laser case are compared. The horizontal bars denote the intervals during which lasing is observed for the transitions designated on the vertical scale, where J is the rotational quantum number of the lower level of the transition. Again, the predictions are nearly identical. This consistency is also observed in the relative energy distributions of the individual vibrational-rotational transitions of the six lasing bands. The amount of information attainable by the use of either model is the same. As demonstrated in the figures, the predictions are very close. The model of Ref. 6 explicitly computes the populations of the individual rotational states. In the present model, this information can be inferred from the calculated transition gains and vibrational populations.

The cost savings achieved by the present model are considerable. For the case described here, the execution time for the Ref. 6 model was 1640 sec on the CDC 7600 computer. For the present model, the time required is just 132 sec. The execution time of the corresponding model without rotational relaxation features[7] is 104 sec. Additional reductions in the present model run time are anticipated as the study progresses.

Since the rotational nonequilibrium model utilizing the technique described herein costs only slightly more to run than the corresponding equilibrium model, laser calculations with rotational relaxation taken into account can now be carried out routinely. Furthermore, parametric studies can be performed that will improve understanding of the importance of rotational relaxation in laser predictions. The technique is applicable to

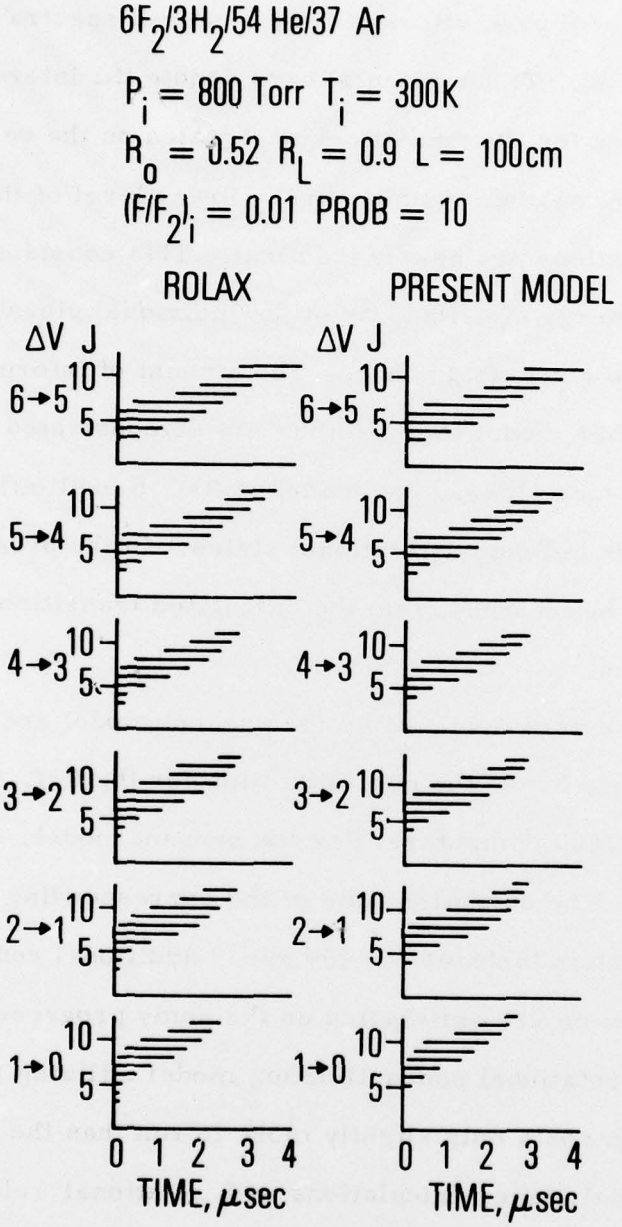

Fig. 2. Comparison of Time-Resolved Spectra of Present Model and ROLAX

both pulsed and cw laser calculations. Of particular interest is its possible application to wave optics modeling of cw laser beam quality, where the added spectral realism afforded by considering rotational nonequilibrium can now be obtained at a much more reasonable cost.

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