Comparison of Rigorous and Simple Vibrational Models for the CO_2 Gasdynamic Laser

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Introduction

OVER the past few years, a number of papers have reported the theoretical small-signal gain in a CO_2 gasdynamic laser. The rate equations that have been used fall into two classes. One group of authors[1-3] has used the rigorous, but complex and nonlinear, equations based on the treatment of Schwartz et al.[4] The second group of authors[5-7] has used a linearized and simplified set of equations. Some justifications for using the simple equations are that they save computation time, are convenient for parameter studies, and sometimes allow analytic solutions to problems. Despite their advantages, the accuracy of the simple rate equations has never been examined carefully. MacDonald[8] questioned their accuracy but did not make any calculations to prove his point. Anderson et al.[5] found good agreement between measured gain and calculations using the simple equations with the generally accepted vibrational rates but made no comparisons with the rigorous equations. On the other hand, other authors[7] have found it necessary to readjust the rates to get agreement between experiment and the simple equations.
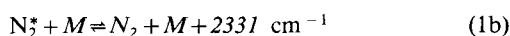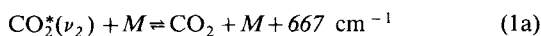
The purpose of this Note is to assess the accuracy of a simple model for computing the gain in a CO_2 gasdynamic laser by comparing computed results from it with computed results from the rigorous model and also with experiment. The comparisons are made with the rates and all other conditions identical so that any differences are due solely to the models. Also, results are compared for several gas mixtures and over a range of stagnation temperature in order to provide a fair test of the simple model.

Theory and Experiment

The conservation equations were used in the standard form presented by Emanuel and Vincenti[9] and are not repeated here. They are subject to the following conditions: the flow is steady, quasi one-dimensional, and inviscid; the fluid is a mixture of CO_2, N_2, He, and H_2O treated as perfect undissociated gases; the rotational modes are fully excited; electronic excitation is neglected; and the vibrational modes in CO_2 and N_2 are treated as harmonic oscillators in Boltzmann distributions with separate vibrational temperatures.

Many possible kinetic reactions exist for the set of vibrational energy modes in the mixture of gases just described. The ones chosen for both models are those recommended by Taylor and Bitterman,[10] and they are as follows:

Translational-Vibrational (T-V) Processes

$$CO_2^*(\nu_2) + M \rightleftharpoons CO_2 + M + 667 \text{ cm}^{-1} \tag{1a}$$

$$N_2^* + M \rightleftharpoons N_2 + M + 2331 \text{ cm}^{-1} \tag{1b}$$

Vibrational-Vibrational (V-V) Processes

$$CO_2(\nu_3)^* + N_2 \rightleftharpoons CO_2 + N_2^* + 18 \text{ cm}^{-1} \tag{1c}$$

$$CO_2(\nu_3)^* + M \rightleftharpoons CO_2(\nu_2)^{***} + M + 416 \text{ cm}^{-1} \tag{1d}$$

Here (ν_1, ν_2, ν_3) are, respectively, the symmetric stretching, the doubly degenerate bending, and the asymmetric stretching modes of CO_2. M is any collision partner in the gas, and the asterisks indicate the quanta of vibrational energy. An additional assumption is that $CO_2(\nu_1)$ and $CO_2(\nu_2)$ are in local equilibrium. The preceding reactions are those chosen by Anderson et al.[5] and Munjee[2] for their analyses. The rigorous model rate equations for reactions (1a-1d) are in the literature,[1-3] and so they are not repeated here.

Consider next the simple model rate equations. The most widely used form is given by Anderson et al.,[5] so it has been used here. Anderson et al. model the vibrational kinetics by grouping the nonequilibrium vibrational degrees of freedom into two modes. Mode I consists of the $CO_2(\nu_1)$ and $CO_2(\nu_2)$ vibrational modes, and mode II consists of the $CO_2(\nu_3)$ and N_2 vibrational modes. The vibrational relaxation of these modes is then described by the equations

$$\frac{d}{dt}(e_{vib})_I = \tau_I^{-1}\left[(e_{vib})_I^{eq} - (e_{vib})_I\right] \tag{2a}$$

$$\frac{d}{dt}(e_{vib})_{II} = \tau_{II}^{-1}\left[(e_{vib})_{II}^{eq} - (e_{vib})_{II}\right] \tag{2b}$$

Here, $(e_{vib})_i^{eq}$ is the equilibrium vibrational energy that would be contained in mode i at the local gas temperature; τ_I and τ_{II} are average vibrational relaxation times[5] that combine all of the detailed relaxation times for reactions (1a-1d). The detailed relaxation times used here for both models are taken as the "best-fit" curves given in Taylor and Bitterman[10] and Sharma.[11]

The previously described conservation and rate equations were integrated, using a standard fourth-order Runge-Kutta method, on an IBM 360 computer. Calculations were made for a two-dimensional wedge nozzle with a throat height of 1.27 mm, a throat radius of 2.54 mm, and a wedge half-angle of 15 deg. The solutions were started with the vibrational energy in equilibrium at the nozzle sonic point. Separate subsonic flow calculations verified this assumption for all cases. As part of the solutions, the homogeneously broadened small-signal gain coefficient also was calculated, using standard methods,[6] for a P(22) branch rotational transition of the $00°1-10°0$ vibrational band of CO_2.

To compare with the theoretical gain results, a few measurements of gain also were made in a shock-tube-heated CO_2 gasdynamic laser utilizing a cold helium driver. Measurements were made at a location 3.9 cm downstream from the throat of the wedge nozzle previously described, where the channel area ratio was 17. The chopped beam from
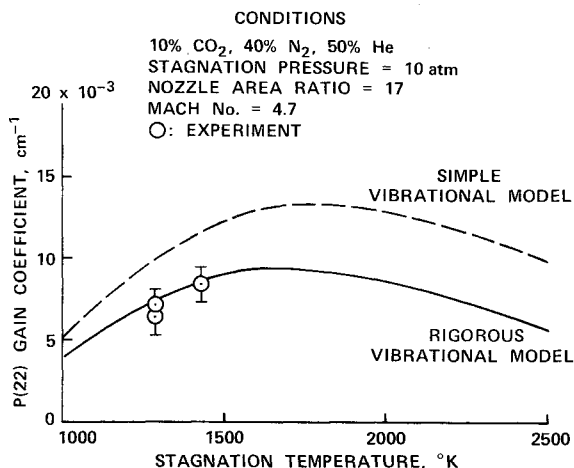

CONDITIONS
10% CO_2, 40% N_2, 50% He
STAGNATION PRESSURE = 10 atm
NOZZLE AREA RATIO = 17
MACH No. = 4.7
O: EXPERIMENT

Fig. 1   Measured and predicted gain coefficient for a wedge nozzle CO_2 gasdynamic laser with 10% CO_2, 40% N_2, and 50% He.
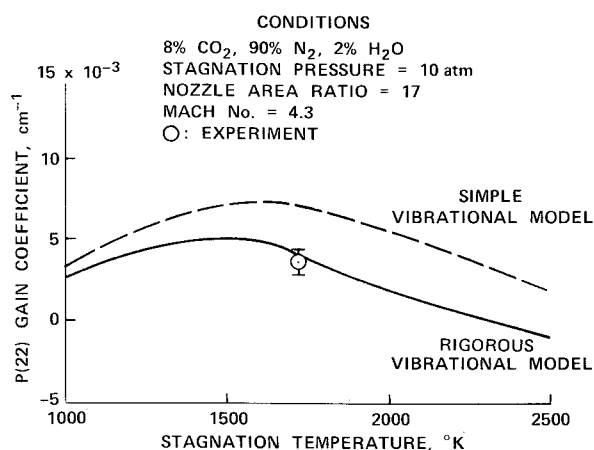
Fig. 2 Measured and predicted gain coefficient for a wedge nozzle CO_2 gasdynamic laser with 8% CO_2, 90% N_2, and 2% H_2O.
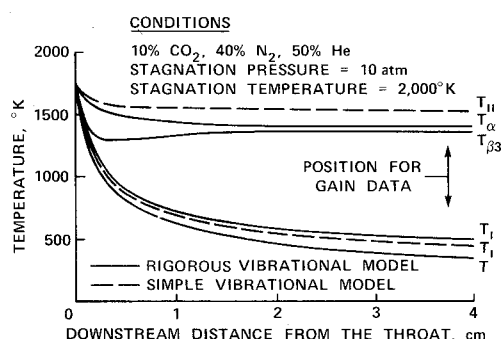

Fig. 3 Gas and vibrational temperatures in a wedge nozzle CO_2 gasdynamic laser for a rigorous and a simple vibrational model [T = gas temperature, $T_I = CO_2(\nu_1,\nu_2)$ vibration temperature (both models), $T_{II} = CO_2(\nu_3)$ and N_2 vibration temperature (simple model), $T_{\beta3} = CO_2(\nu_3)$ vibration temperature (rigorous model), and $T_\alpha = N_2$ vibration temperature (rigorous model)].

a commercial probe laser operating on the P(22) transition was passed through germanium windows located across the 15.2-cm-wide laser cavity. A gold-doped germanium infrared detector, coupled to an oscilloscope, measured the change in beam intensity during a test. This, in turn, was related to the gain coefficient through Lambert's law.[5]

Results and Discussion

The small-signal gain coefficient is presented for a CO_2:N_2:He gas mixture in Fig. 1 and for a CO_2:N_2:H_2O mixture in Fig. 2. Results are shown for the rigorous and simple vibrational models and from experiment. The theoretical data are given over a range of stagnation temperature. The error bars show the estimated experimental uncertainty. The data for both of these mixtures show the rigorous model predicting the experiment quite well, with the simple model consistently predicting too high a gain. Note that the simple model error increases at the higher stagnation temperature, which is where most present-day CO_2 gasdynamic lasers are operated.[12] Although not shown here, several other mixtures produced similar results.

To understand the preceding differences between the two models, consider in Fig. 3 the vibrational temperature distributions in the nozzle for the mixture of Fig. 1 at a stagnation temperature of 2000 K. With reference to the vibrational energy level diagram shown in Fig. 2 of Ref. 5, T is the gas temperature, and T_I, T_{II}, $T_{\beta3}$, T_α are, respectively, the vibrational temperatures of $CO_2(\nu_1,\nu_2)$ for either model, of $CO_2(\nu_3)$ and N_2 for the simple model, of $CO_2(\nu_3)$ for the rigorous model, and of N_2 for the rigorous model. Note that T_{II} is considerably higher than T_α and $T_{\beta3}$, that T_α and $T_{\beta3}$

do not equal each other as assumed in the simple model, and that T_I is lower for the simple model than it is for the rigorous model. All of these differences contribute toward making the simple model gain higher. These observations are typical for the other cases computed here also.

Through examination of the computer results from the two vibrational models, the causes of the preceding errors for the simple model have been identified. First of all, T_{II} is too high because Eq. (2b) underestimates the true "driving potential" deactivating $CO_2(\nu_3)$ and N_2 through reaction (1d). The error can exceed an order of magnitude at the high temperatures near the throat, where these modes usually "freeze out." Second, T_α and $T_{\beta3}$ are not equal because the finite rate for reaction (1c) allows $T_{\beta3}$ to be "pulled" below T_α through reaction (1d) near the throat. Although further downstream the two modes do achieve "local equilibrium" with each other, they continue to maintain a temperature difference caused by a combination of their quantum energy mismatch and the low gas temperature.[13] Finally, T_I for the simple model ends up too low because Eq. (2a) ignores the energy being pumped into $CO_2(\nu_2)$ through reaction (1d) and also erroneously includes $CO_2(\nu_1)$ along with $CO_2(\nu_2)$ in the "driving potential" for reaction (1a).

To summarize, in this study we have computed the gain in a CO_2 gasdynamic laser using both a simple vibrational model and a rigorous model. The two models agree fairly well at low temperatures, but the simple model predicts too high a gain at the higher temperatures of current interest. By manipulating the vibrational relaxation times, one can force the simple model to agree with a particular set of experimental data, and some authors have done this successfully. However, the present results suggest that this may not be accurate for other temperatures, mixtures, or geometries.

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