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Parametric Study of DF–CO_2 Transfer Chemical Laser by the Numerical Model Simulation

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The effects of the concentration and the pressure of reactants on laser output were reported in the previous study. The present study is made of the following main parameters on laser characteristics; the initial temperature of the reaction mixture, inert gas (He) added in the reaction mixture, and the level of initiation as a function of time. As the initial temperature of reaction mixture decreases, both the output energy and the duration time increase. Especially, the output energy is linearly proportional to the inverse of the initial temperature. In order to obtain a proper lasing for a given condition, a sufficient amount of He must be added: The optimum ratio of [He] to $[D_2 + F_2 + CO_2]$ is found to be greater than 2. In addition, the time dependence of level of initiation (TDLI) shows no significant difference in total output energy from that of the premixed model, but only the power profile.

Introduction

A DF–CO_2 transfer chemical laser (TCL) is a type of CO_2 laser which releases a high power of 10.6 μm beam. While in the conventional CO_2 laser the N_2 gas added plays a central role to improve the lasing efficiency[1], in TCL the function of N_2 is replaced with the excited DF molecules[2]. Namely, it achieves a population inversion of CO_2 by the vibrational energy transfer of excited DF molecules formed by $(D_2 + F_2)$ chain chemical reactions. Since the population inversion of CO_2 is achieved from the chemical reactions, the phenomena occurring in this laser system are very complicated[2]. In order to get a better understanding of the mechanism of how the laser operates, model simulations of this system have the developed extensively[3-11]. We reported the results of the calculation of power in which show[12] good agreement between the previous experimental and theoretical studies reported in the literature. Additionally, we discussed the optimum lasing conditions for the initial concentration ratios of reaction mixture (D_2:F_2:CO_2:He) by comparing the result of the experiment with the calculation. However, there are various important other aspects in the operation of the DF–CO_2 TCL, which have been reported little in the literature. These include the role of the initial temperature of reaction mixture to lasing efficiency and energy; the role of added inert He gas in the reaction mixture; the change of laser characteristics such as intensity and duration profile, governed by the duration of the reaction-initiating pulse.

In general, oscillation takes place between two vibrational levels of (00°1) and (10°0) in CO_2 laser[13]. To obtain a strong laser action, the (00°1) level must be over-populated. Note that an increased temperature of reaction mixture suppresses the power releasing followed by a rising population of (10°0) level. However, only a few reports are available on detailed results of systematic theoretical calculations for this laser (TCL). First, we describe the effects of initial temperature of the reaction mixture at several conditions.

The reaction mixture of DF–CO_2 TCL often contains the

inert gas He so that addition of He gas tends to depopulate the (10°0) level by collision and helps to keep the CO_2 cold by conduction of heat away to the walls[14]. The optimum ratio of He to the other reaction components will be investigated by calculating the lasing power and efficiency.

On the other hand, $D_2 + F_2$ chain reactions are initiated by the F radicals generated from F_2. The initiation ratio of F, $[F]/[F_2]_o$, is often defined as the level of initiation. In experiment the various methods are used to initiate the reaction; initiation by flash lamps, the radiation from high-currents open discharge, and electron beam.[15] Therefore, the degree of initiation depends on the characteristics of various initiation methods. Particularly, in photoinitiation systems the generating rate (or ratio) of the F radicals is strongly affected by the intensity and the time of duration in flash lamp which is used for initiating the chain reaction. In model simulations, this value has been assumed to be constant[3,4] in premixed model or a simple function of time[15,16]. The premixed model is a simple assumption to make the power calculation easy so that it has been used to many researchers[3,4] including us[12]. However, for the practical power calculation careful consideration of the assumption should be made. In the present work we will investigate the difference of the results of both assumptions, the premixed model and the model with time dependence of level of initiation (TDLI). We research that these two models take different viewpoints to the characteristics of the laser light.

Initial Conditions and Calculations

Firstly, to study the effect of initial temperature on the laser power, we perform calculations at several temperature varing from 200 K to 500 K by 50 K interval at 5 different pressures (50, 190, 250, 380 and 760 torr). Secondly, to examine the effect of inert gas (He) on leasing the power and efficiency of laser is calculated at 380 torr and 300 K. In this calculation that ratio of D_2:F_2:CO_2 is fixed at 4:4:20 which is the optimum ratio according to our previous result[12]. With the constant total pressure of 380 torr, only the ratio of He is varied from 10 to 200 for 10 different points, i.e. D_2:F_2:CO_2:He = 4:4:20:x, x = 10, 20, 30, 40, 50, 60, 70, 150 and 200. The final item of this study is the level of initiation. As metioned before, we define the level of initiation as the ratio of $[F]/[F_2]_o$, i.e., the amount of F radicals consumed during the lasing. The generating rate of F radicals by photoinitiation can be expressed by the modified Gaussian profile as[15].

$$d[F]/dt = 2\gamma t \exp(-t/t_o)[F_2]_o$$

where

t : time
γ : parameter calculated with the intensity of flash lamp
t_o : half the maximum duration of flash lamp

Given the generating rate of F radicals, the level of initiation for the TDLI model can be integrated as,

$$[F]/[F_2]_o = 2\int_0^{t_c} \gamma\, t \exp(-t/t_o)\, dt$$

$$= 2\gamma\, t_o^2 [1 - (1 + t_c/t_o) \exp(-t_c/t_o)]$$

Table 1. Parameters Used to Investigate the Effect of Level of Initiation for Total Pressures of 50, 190, 380 and 760 Torr

Case	t_o (μsec)	γ
a	5.5×10^{-1}	1.65×10^{10}
b	3.3	4.79×10^{8}
c	5.5	1.93×10^{8}
d	5.5×10^{1}	1.70×10^{8}

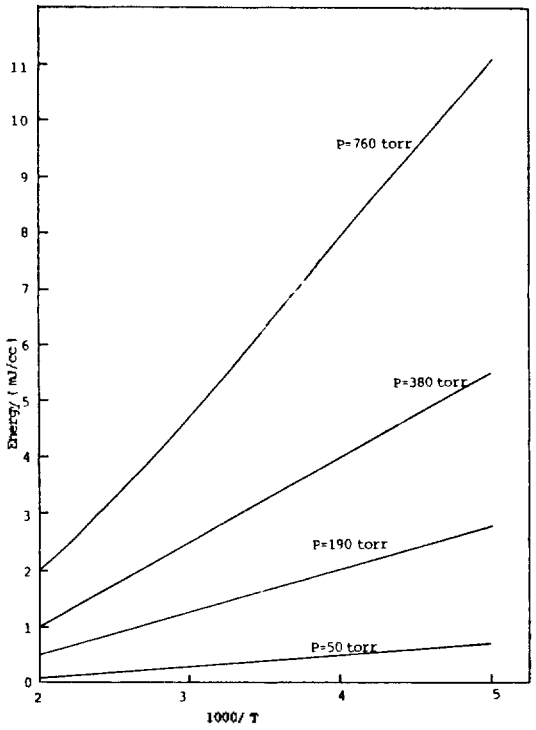

Figure 1. Effect of initial temperature of reactants on laser energy. D_2:$F_2$$CO_2$:He = 1:1:6:19.

where t_c is the duration time of the laser. To compare the TDLI with the premixed model, we carry out calculations at 4 different conditions listed on Table 1 by changing the intensity (γ) and duration (t_o) of flash lamp with the level of initiation fixed at 0.01.

Results and Discusion

The Effect of Initial Temperature. The effects of initial temperature varing from 200 K to 500 K at four total pressures with a fixed level of initiation and a mixing ratio are depicted in Figures 1 and 2 for the output energy and the duration time, respectively. They show that the output energy and the duration time of lasing are increased as the initial temperature decreases. Particularly, the output energy shows a linear response to the inverse of the temperature. The increasing tendency of the energy on the temperature decrement has been also reported by many researchers[6,7,9]. For extreme conditions such as a very low level of initiation and a very high pressure with O_2 added, however, they have found from their calculation[9] that the cooling of the mixture does not improve the output energy.

On the other hand, the linear relationship of the output

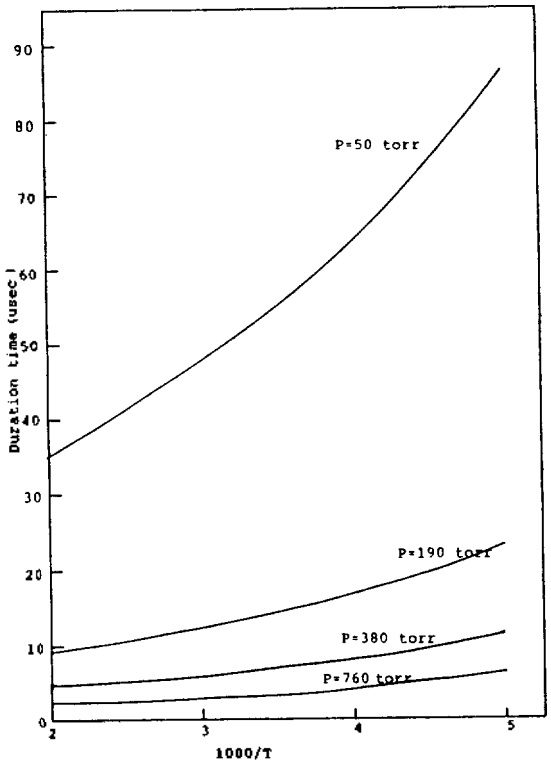

Figure 2. Effect of initial temperature of reactants on duration time. $D_2 : F_2 : CO_2 : He = 1 : 1 : 6 : 19$.

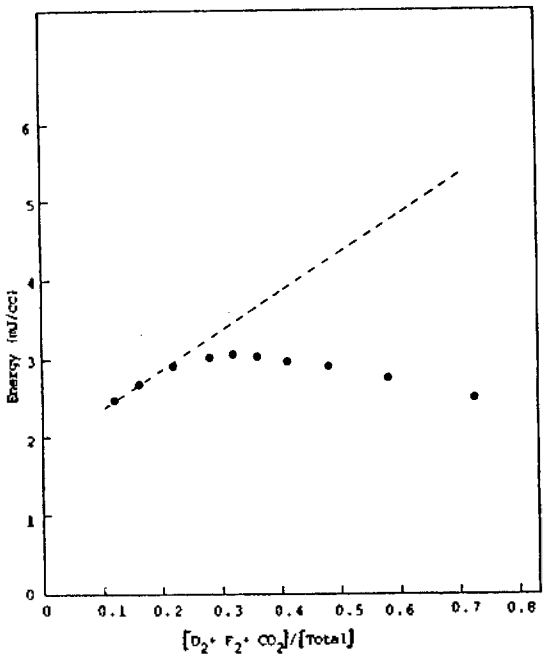

Figure 3. Effect of inert gas on laser energy at constant total pressure of 380 torr. The data points indicates the $D_2 : F_2 : CO_2 : He = 4 : 4 : 20 : x$, x = 200, 150, 70, 60, 50, 40, 30, 20 and 10.

energy on pressure variation has been also reported by many groups[4,6,7,9,12]. It is easy to show that both pressure and the inverse of the temperature have a linear relationship to the molar density of the mixture according to the ideal gas law. Therefore, the output energy seems to be directly related to the amounts(mole) of the reactants in usual conditions, at least, in a qualitative sense. For the Boltzmann distribution and chemical kinetic rate which contain the exponetial temperature terms, the temperature effect by these on laser output seems to be minor factor compared with that of the increment of molar density.

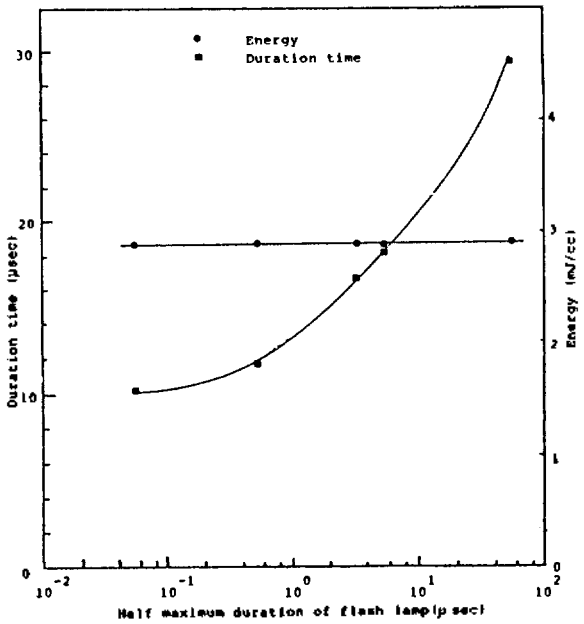

Figure 4. Effect of half maximum duration of flash lamp on the laser output energy and duration time. $D_2:F_2CO_2He = 1:1:6:19$ with constant total pressure of 250 torr.

The Effect of He as a Diluent. It is obvious that He gas does not produce a direct chemical effect on laser power. However, the addition of He keeps the gas mixture cool and depopulates the lower laser level of $CO_2(10°0)$ by collision. Thus, He is necessary to achieve a proper lasing performance. Figure 3 shows the output energy *vs.* the ratio of $[D_2 + F_2 + CO_2]/[D_2 + F_2 + CO_2 + He]$ at constant total pressure. It is notable that a monotonic increment of energy is not observed as the reactants($[D_2 + F_2 + CO_2]$) are increased. When the He content is large enough,but the ratio is below 0.25 there is a linear increment (the dotted line in the figure) between the energy and the amount of reactants. On the other hand, at the ratio at or above 0.25, the output energy decreases inspite of the increament in reactants. This indicates that He must be added sufficently to have the proper lasing; in most experimental work[3,11] He is added more than two times of reactants mixture.

Time Dependence of Level of Initiation (TDLI). In order to observe the effect of TDLI on the laser power and the duration time we have performed calculations with the conditions of Table 1 at a constant pressure (250 torr). The effect of a half the maximum duration of flash lamp on the laser output energy and the duration time is depicted in Figure 4. As the duration of flash lamp (t_o) increases, the duration time of laser also increases, while the energy remains constant within 1%. Figure 5 shows that the power profile depends on the flash lamp condition, demonstrating another aspect already seen on Figure 4. An increase in the duration of flash lamp delays the generation of laser power : that is, it makes the peak power lower and the duration time longer. However, the area of the peak curve, which cor-

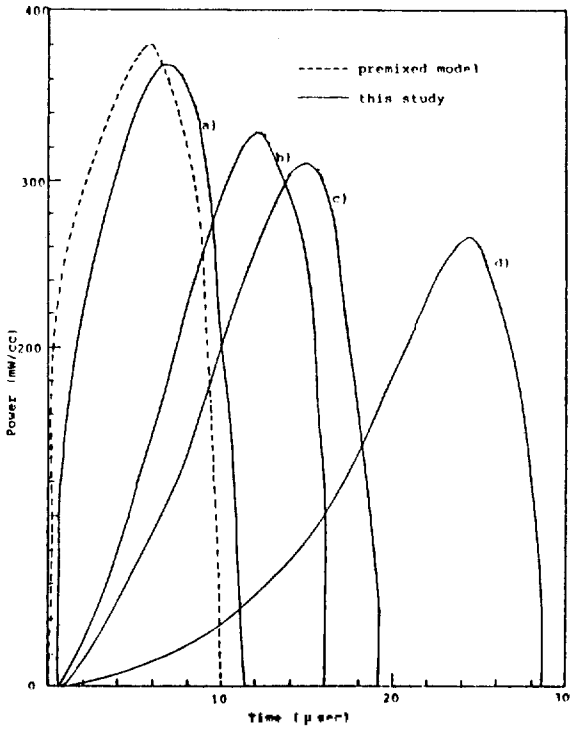

Figure 5. Power profile at the various flash lamp condition. t_0(μsec) ; a) 5.5×10^{-1}, b) 3.3, c) 5.5, d)5.5×10^{1}
$D_2 : F_2 : CO_2 : He$ = 1: 1: 6: 19 with constant total pressure of 250 torr.

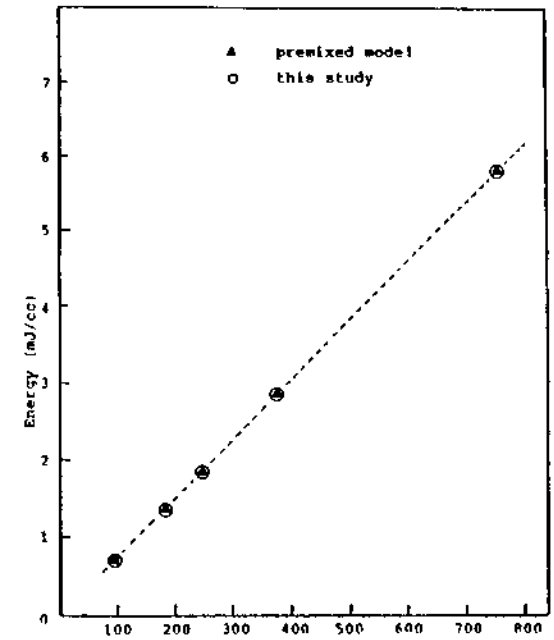

Figure 6. The dependence of output energy on total pressure of reactants. $D_2 : F_2 : CO_2 : He$ = 1: 1: 6: 19, T = 300 K.

responds to the lasing energy, does not change significantly at a fixed level of initiation.

To consider the pressure dependence of the difference between the premixed model and TDLI, we carry out the calculations for four different total pressures (190, 250, 380 and 760 torr) at fixed level of initiation, 0.01. The results are displayed in Figure 6 and demonstrated the linear dependence of the laser energy on the total pressure for both models. As a consequence of good agreement of the premixed model with TDLI, it is noteworthy that the premixed model is a crude approximation but reasonable assumption.

Conclusion

Through these parametric study some significant conclusions seem to be reached. As the initial temperature of reaction mixture decreases, both the output power energy and duration time of laser increases. Particularly, the output power shows a linear relation to inverse of initial temperature. Considering the effect of He, He must be added sufficiently to provide the energy high enough for a given condition. Namely, the ratio of $[He]/[D_2+F_2+CO_2]$ is found to be greater than 2. The time dependence of the level of initiation (TDLI) shows no significant difference in total output energy from that of the premixed model, but only the power profile. The duration time of laser is increased with the increment of half maximum duration of flash lamp (t_0) for the fixed level of initiation. Therefore to obtain the efficient laser beam such as high peak power and short duration time, the duration of flash lamp must be kept short and its intensity should be high.

Acknowledgement. This research was supported by the Korean Science and Engeering Foundation(KOSEF).

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