

## HF 화학 레이저에 대한 Model Simulation과 그 작동 특성의 수치분석

金良美·金 熊\*·趙雄仁†

연세대학교 이과대학 화학과

\*연세대학교 이과대학 물리학과

(1988. 8. 2 접수)

### Model Simulation of a HF Chemical Laser and Numerical Analyses of It's Behaviors

Yang Mee Kim, Ung Kim\*, and Ung-In Cho†

Department of Chemistry, Yonsei University, Seoul 120 - 749, Korea

\*Department of Physics, Yonsei University, Seoul 120 - 749, Korea

(Received August 2, 1988)

**요 약.** 화학 레이저 모델의 이론적 연구를 화학 반응속도론, gain 과정과 유도 방출과정을 고려하여 수행하였다. 우선  $F+H_2$  비 연쇄반응 HF 화학 레이저를 진동준위가  $v=3$ 까지 pumping 되는 것으로 생각하고 관련된 rate equation을 풀어서 출력을 산출하였다. 여기서 조화진동자를 가정한 계산과 비조화성 보정을 해준 계산결과와 비교로부터 그 차이가 거의 없음을 확인하였다. 또한 여러가지 온도와 초기농도를 택하여 산출되는 laser 출력의 변화를 검토하였다. 그리고  $H_2 + F_2$  연쇄반응 HF 화학 레이저에 관한 비교적 단순한 model simulation을 수행하였다. 이 계산결과는 이미 보고된 상당히 복잡한 계산결과와 비교하여 만족할 정도이었다.

**ABSTRACT.** Theoretical analysis of HF chemical laser models are performed through chemical reaction kinetics, gain process and stimulated emission process. A chemical laser of  $F + H_2$  nonchain reaction is investigated through V-R transitions of excited HF for vibrational levels up to  $v = 3$  and rate equations including non-chain pumping and deactivation. On this analysis, harmonic and anharmonic vibrational levels are considered separately and the results of the corresponding power calculations are showed very small difference between the two. Output powers are calculated with variation of temperature and initial concentrations of  $H_2$ . A HF chemical laser of  $H_2 + F_2$  chain reaction is also simulated with a premixed initial condition. Results of present model calculations are satisfactory through comparison with detailed calculations reported by others.

### 1. INTRODUCTION

A chemical laser<sup>1</sup>, where the population inversion is produced directly or indirectly by an exothermic chemical reaction, is of great interest for two main reasons: First, it provides a direct conversion of chemical energy into electromagnetic energy. Second, one can expect high output power due to available large energy in a chemical reaction. Since Kasper and Pimetal realized a chemical

laser for the first time in 1965,<sup>2</sup> numerous types of chemical lasers have been investigated experimentally. Meanwhile the theoretical investigations have been progressed significantly. After Cohen *et al.*<sup>3</sup> firstly attempted computer simulation of a chemical laser in 1969, Airey<sup>4</sup> modeled  $Cl + HBr$  pulse laser and succeeded in the calculation of the laser power as a function of time.

Emanuel<sup>5</sup> attempted a simplified theoretical analysis of a continuous wave chemical laser with

vibrational-rotational transition between two vibrational levels of a hypothetical diatomic molecule. New features in this study included an analysis of J-shifting in which lasing shifts from one rotational level to the next level. And shortly after, he extended<sup>6</sup> his analytical model to a HF chemical laser by  $F + H_2$  non-chain reaction, with considering first three bands  $1 \rightarrow 0$ ,  $2 \rightarrow 1$ , and  $3 \rightarrow 2$  in vibrational transitions. His group continued to develop computer simulation code of a pulsed HF laser to  $H_2 + F_2$  chain reaction system.<sup>7-8</sup> The systems were considered chemical kinetics with sixty-eight reactions and calculated the laser power from the first six-vibrational level of HF as a function of time. Besides these, other groups have tried computer simulations of chemical lasers, such as  $DF/CO_2$ ,<sup>9-11</sup>  $H_2/F_2/O_2$ ,<sup>12</sup> and  $DF/O_2/CO_2$ <sup>13,14</sup> systems.

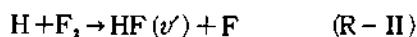
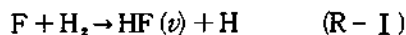
Hydrogen halide systems have been studied most extensively among many chemical laser systems, due to their highly exothermicities and large electric dipole moment. Among hydrogen halide systems, HF chemical laser has the largest pumping efficiency and has been studied most intensively. As a consequence, the present study will be modeled HF chemical laser system.

To understand a chemical laser fully, one has to know three disciplines; chemical kinetics of non-equilibrium reactions, gas dynamics of reactive flows, and laser physics of high-gain media. However, the major investigation in the present model is limited to chemical kinetics. For other disciplines, only simple assumptions will be used.

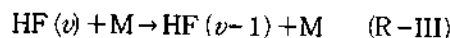
## 2. THEORETICAL BACKGROUND

**2.1 Chemical Kinetics.** The reaction mechanism for HF chemical laser system can be represented by pumping reactions, deactivation processes, exchange processes, and emission processes:

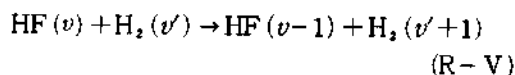
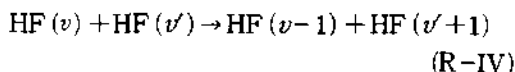
(1)  $H_2 + F_2$  chain (pumping) reactions;



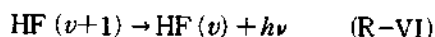
(2) Vibrational-translational (V-T) deactivations;



(3) Vibrational-vibrational (V-V) exchanges;



(4) Stimulated emissions;



In the pumping reactions of (R-I) and (R-II), the F-atom, which has large electronegativity, reacts with  $H_2$  and produces excited  $HF(v)$  and H-atom. And this H-atom reacts with  $F_2$  and produces another excited  $HF(v')$  and F-atom. Thus the chain reactions occur. While the (R-I) produces  $HF(v)$  of  $v = 0, 1, 2, 3$ , the  $HF(v')$  of states from  $v' = 0$  to  $v' = 9$  are obtained by (R-II). However the excited  $HF(v)$  above  $v = 4$  is known to have very small contribution to lasing due to the reverse reaction of (R-I) and other deactivation reactions. When only (R-I) is considered, it is called non-chain reaction and is corresponded to the reactions between  $H_2$  and inorganic fluoride compounds, such as  $CF_4$ ,  $UF_6$ ,  $SF_6$  and  $MoF_6$ .

The output power of HF laser depends on the initial concentration of F-atom in both chain and non-chain reactions. Thus the initiation process producing F-atom is very important. However present analysis is not related to a specific initiation process. A premixed model, in which an initial concentration of F-atom is assumed to be given, will be used for the present calculations.

The vibrational distributions of the excited  $HF(v)$  produced from (R-I) and (R-II) are much greater than the corresponding Boltzmann distribution. Thus the pumping efficiency is known to be larger than other hydrogen halides. The rate constants of (R-I) and (R-II) for  $v = 0, 1, 2, 3$  are shown as (R-1) and (R-2) respectively in Table 1 and the relative distributions for each vibrational

Table 1. Kinetic model for H<sub>2</sub> + F<sub>2</sub> laser

Reaction no.	Reaction	Rate coefficient	Distribution constant $\alpha(v)$			
			$v=0$	1	2	3
R-1	F + H <sub>2</sub> ⇌ HF(v) + H	$k_1 = 1.62 \times 10^{14} e^{-1600/RT}$	0.056	0.011	0.555	0.278
R-2	H + F <sub>2</sub> ⇌ HF(v) + F	$k_2 = 3.7 \times 10^{13} e^{-2400/RT}$	0.162	0.162	0.243	0.433
R-3	HF(v) + HF ⇌ HF(v-1) + HF	$k_{HF} = 6 \times 10^{16} T^{-1.43}$	0	0.167	0.333	0.500
R-4	HF(v) + H <sub>2</sub> ⇌ HF(v-1) + H <sub>2</sub>	$k_{H_2} = 8.3 \times 10^5 T^{2.2} e^{-562/RT}$	0	0.965	0.035	0
R-5	HF(v) + F ⇌ HF(v-1) + F	$k_F = 5.4 \times 10^9 T^{1.3}$	0	0.167	0.333	0.500
R-6	2HF(v) ⇌ HF(v-1) + HF(v+1)	$k_{2HF} = 4.0 \times 10^5 T^{2.2}$	0	0.333	0.333	0.333
R-7	F + H <sub>2</sub> ⇌ HF(v) + H	$k_{1(v)} = 10^{12} T^{0.670}$	$v = 4 \sim 6$			
R-8	H + F <sub>2</sub> ⇌ HF(v) + F	$k_{2(v)} = a_4 k_2$	$a_4 = 10/3, a_5 = 11/2, a_6 = 5$			

\* All rate coefficients are in cm<sup>3</sup>/mole-sec, and  $R = 1.987$  cal/mole-K and chosen selectively from ref. 7.

level are listed as  $a_0, a_1, a_2, a_3$  at the right side of the Table 1. For higher vibrational states above  $v=4, 5, 6$ , forward reaction of the rate constants of (R-II) and reverse reaction of (R-I) are separately shown as (R-8) and (R-7) respectively in the Table 1. It is worth while to note that the  $a_2$  of (R- ) is greater than 0.5 and  $k_1$  is much greater than  $k_2$ . This means that the major contribution of HF laser comes from (2 → 1) transition.

The next processes, (R-III), (R-IV) and (R-V) are deactivation processes, where the excited HF(v) is losing its energy by collision with other molecules. Beside the processes, other reactions are excluded due to negligible contribution to the laser pumping. The rate constants as a function of temperature for each reaction are listed in Table 1. These correspond to 30 reactions among 68 reactions which were suggested for the simulation of HF laser by Kerber and Emanuel.<sup>7</sup>

**2.2 Gain.** The gain coefficient in rotational-vibrational transition is expressed in terms of transition probability and population difference between levels. When the rotational population of a Boltzmann distribution and only P-branch transition are assumed, the gain coefficient between  $(v+1)$  and  $v$  vibrational state is given by<sup>7</sup>

$$\alpha(V, J) = \frac{hN_A}{4\pi} \omega_c(V, J) \Phi(V, J) \rho B(V, J) \cdot (2J+1) \left\{ \frac{n(v+1)}{Q_r(v+1)} \right\} \cdot \exp\left(-\frac{hcE(v+1, J-1)}{kT}\right)$$

$$- \frac{n(v)}{Q_r(v)} \exp\left(-\frac{hcE(v, J)}{kT}\right) \} \quad (1)$$

where  $h$  is the Planck's constant,  $N_A$  is the Avogadro number,  $\rho$  is density,  $J$  is rotational level, and  $n(v)$  is mole-fraction at  $v$  vibrational level. And  $\omega_c$  is the transition frequency in wave number,  $\Phi$  is the line profile,  $B$  is the Einstein coefficient, and  $Q_r$  is the rotational partition function. These are given in the followings:

$$\omega_c(v, J) = G(v+1) - G(v) + E(v+1, J+1) - E(v, J) \quad (2)$$

$$G(v) = \sum_{j=1}^{\infty} Y_{j0}(v+1/2)^j \quad (3)$$

$$E(v, J) = \sum_{j=1}^{\infty} \sum_{l=0}^{\infty} Y_{jl}(v+1/2)^j (J(J+1))^l \quad (4)$$

$$\Phi_{DP} = (\ln 2/\pi) / \alpha_{DP}(v, J) \quad (5)$$

$$= [2.0 \times 10^7 N_A k \ln 2 / c^2]^{1/2} \omega_c(v, J) (T/M)^{1/2} \quad (6)$$

$$B(v, J) = \frac{16\pi^4 \times 10^{-7}}{3h^3 c} \left(\frac{2J}{2J+1}\right) M(v)^2 \quad (7)$$

$$Q_r = 1 + \sum_{j=1}^{\infty} (2j+1) \exp(-hcE(v, J)/kT) \quad (8)$$

$$\cong T/\sigma\theta_r, \quad \sigma; \text{ symmetry factor} \quad (9)$$

$$\theta_r = (hc/k) Y_{01} + Y_{11}(v+1/2) \quad (10)$$

Here vibrational energy,  $G(v)$  and rotational energy  $E(v, J)$  can be given in terms of Dunham coefficients,<sup>8</sup>  $Y_{ij}$ , which include anharmonic corrections. However, for the HF system the anharmonicity in low vibrational levels are very small due to deep potential well. And line-profile  $\Phi_{DP}$  is

assumed Doppler broadening.<sup>15</sup> Einstein coefficient,  $B(v, J)$ , is the transition probability between two states.<sup>16</sup> This coefficient is proportional to the square of the matrix element of the electric dipole moment whose value is taken from polynomial expansion for RKR potential.<sup>17</sup>

With assuming harmonic oscillator, the gain coefficient can be expressed<sup>5</sup> very simply as following;

$$\alpha_n = \alpha_r(v) f \exp(- (J^2 - J) \delta) [n(v+1) - n(v) \exp(-2J\delta)]$$

$$\alpha_r(v) = 2.74 \times 10^{47} \sigma \theta_r \omega^{1/2} T^{-3/2} \rho |M(v)|^2$$

$$\delta = \theta_r / T \quad (12)$$

**2.3 Stimulated Emission.** To occur lasing the gain coefficient  $\alpha$ , given by either Eq. (1) or Eq. (11), should be greater than or equal to a certain threshold value. According to a steady-state condition, gain-equals-loss condition, the threshold gain is given by,

$$\alpha_{th} = -\ln(r_r r_L) / 2L \quad (13)$$

where  $L$  is distance between lasing medium, and  $r_r$  and  $r_L$  are the reflectivities of the mirrors located right and left side. When the  $\alpha_{th}$  is large, the chance to occur lasing will be reduced. In the limit of  $L = \infty$  or  $r_r r_L = 1$ ,  $\alpha_{th}$  will be zero and consequently one can count on lasing whenever the vibrational distribution is over the equilibrium, Boltzmann distribution. When  $\alpha_{th}$  from Eq. (13) is compared with  $\alpha$  value from either Eq. (1) or Eq. (11), one can figure out whether the lasing in (R-VI) is available or not.

Now, the concentration rate of excited HF( $v$ ) can be thought as products from chemical reaction and lasing process,

$$\rho \frac{dn(v)}{dt} = R_c(v) + R_r(v) - R_r(v-1) \quad (14)$$

where  $R_c(v)$  is the concentration rate of HF( $v$ ) produced through chemical reactions,  $R_r(v)$  is the production rate of  $v$ -vibrational state due to the lasing from  $v+1$  to  $v$  state. And the output power is given by

$$P_1(t) = \sum_{v=0}^{v_r-1} N_A h \cdot c \omega_c(v, J) \cdot R_r(v, J) \quad (15)$$

where  $v_r$  is the available maximum vibrational state of lasing. To know  $R_r(v)$ , one has to evaluate  $dn(v)/dt$ . This can be obtained from coupled differential equations of equation of state and equations of motion which are conservation laws of mass, momentum and energy, in addition to the chemical rate equations. However the process is required all the thermodynamic data of each chemical species besides lots of computing time. Therefore the present calculation prefer simpler model which will be discussed later. It is noted that when  $\alpha < \alpha_{th}$ ,  $R_r(v) = 0$ ,  $n(v)$  can be obtained directly from  $R_c(v)$ , and when  $\alpha > \alpha_{th}$ ,  $R_r(v)$  is got from  $dn(v)/dt$  with assuming  $\alpha = \alpha_{th}$ .

### 3. THE MODEL OF CHEMICAL LASER

**3.1 Non-Chain HF Chemical Laser.** The non-chain reaction, *i.e.*, without (R-II) reaction can be treated relatively simply. The gain coefficient from Eq. (1) or (11) can be used to calculate concentrations of each vibrational level by gain-equals-loss condition, as

$$-\ln(r_r r_L) / 2L = An(v+1) - Bn(v) \quad (16)$$

where  $A$  and  $B$  can be evaluated from Eq. (1) or (11). Thus  $n(1)$ ,  $n(2)$  and  $n(3)$  can be expressed in terms of  $n(0)$  or  $n_r = (0) + n(1) + n(2) + n(3)$  according to Eq. (16).

In the meantime,  $R_r(v)$  in Eq. (14) can be obtained from Table 1, if one knows concentrations of each species involved as,

$$R_c(v) = \rho^2 \{ k_1 a_1(v) [F] [H_2] + k_{HF} [HF] \{ a_{HF}(v+1) n(v+1) - a_{HF}(v) n(v) \} + k_{H_2} [H_2] \{ a_{H_2}(v+1) n(v+1) - a_{H_2}(v) n(v) \} + k_F [F] \{ a_F(v+1) n(v+1) - a_F(v) n(v) \} + k_{MHF} \{ a_{MHF}(v+1) n^2(v+1) - 2a_{MHF}(v) n^2(v) + a_{MHF}(v-1) n^2(v-1) \} \} \quad (17)$$

And the concentrations can be calculated from followings:

Since

$$-\frac{d}{dt}[\text{F}] = \frac{d}{dt}[\text{HF}] = k_1 \rho [\text{F}] [\text{H}_2] \\ = k_1 \rho [\text{F}] \{[\text{H}_2]_0 - [\text{F}]_0 + [\text{F}]\} \quad (18)$$

[F] is given by,

$$[\text{F}] = [\text{F}]_0 (1 - K) e^{-t/\tau} / (1 - Ke^{-t/\tau}) \quad (19)$$

where

$$K = [\text{F}]_0 / [\text{H}_2]_0 \\ \tau^{-1} = k_1 \rho \{[\text{H}_2]_0 - [\text{F}]_0\}$$

Thus

$$[\text{HF}] = [\text{HF}]_0 + [\text{F}]_0 - [\text{F}] \\ [\text{H}] = [\text{H}]_0 + [\text{F}]_0 - [\text{F}] \\ [\text{H}_2] = [\text{H}_2]_0 - [\text{F}]_0 + [\text{F}] \quad (20)$$

It is worthwhile to note that [F] is approximately decreasing as  $\exp(-t/\tau)$  when  $[\text{H}_2]_0 \gg [\text{F}]_0$ . Now one can compute  $R_s(\nu)$  in Eq. 15 very simply using  $n_i = [\text{HF}]$ , and thus the output power  $P_s(t)$  with assuming Boltzmann distribution in rotational population and the  $J$ -shift for maximum gain.

**3.2 Chain HF Chemical Laser.** The pumping mechanism in the chain reaction are involved by (R-I) and (R-II). From the both reactions, the HF is produced continuously and atomic F and H are produced and consumed. In Table 1, (R-7) is the reverse reaction of (R-I) and (R-8) is the forward reaction of (R-II) for high vibrational level of HF( $\nu$ ),  $\nu=4,5,6$ . The reason why the (R-7) and (R-8) are considered separately from (R-2) is that as the highly excited HF( $\nu$ )s above  $\nu=4$  is produced from (R-8), the molecules are attacked by H atoms before deactivation or lasing process is occurred. Consequently, the contributions to lasing for the highly excited HF( $\nu$ ) above  $\nu=4$  are known to be very small. Thus the present model is limited the lasing species to HF(0), HF(1), HF(2) and HF(3).

To solve the rate equations for this chain reactions, the HF molecules from (R-1), (R-2) and (R-8) is expressed as HF1, HF2 and HF3, respectively, and F atoms from (R-7) as F1 separately, for distinction. Then necessary rate equations would be written as followings,

$$d(\text{HF1})/dt = k_1 \rho [\text{F}] [\text{H}_2]$$

$$d(\text{HF2})/dt = k_2 \rho [\text{H}] [\text{F}_2] \\ d(\text{HF3})/dt = k_3 \rho [\text{H}] [\text{F}_2] - k_7 \rho [\text{HF3}] [\text{H}] \\ d(\text{F1})/dt = k_7 \rho [\text{HF3}] [\text{H}] \quad (21)$$

And the concentrations of each species are given by

$$[\text{F}] = [\text{F}]_0 - [\text{HF1}] + [\text{HF2}] + [\text{HF3}] + 2[\text{F1}] \\ [\text{H}_2] = [\text{H}_2]_0 - [\text{HF1}] + [\text{F1}] \\ [\text{H}] = [\text{HF1}] - [\text{HF2}] - [\text{HF3}] - 2[\text{F1}] \\ [\text{F}_2] = [\text{F}_2]_0 - [\text{HF2}] - [\text{HF3}] - [\text{F1}] \quad (22)$$

Since the rate equations of Eq. (21) are coupled differential equations, it can be solved by Runge-Kutta-Gill method. Of course, one more equation for temperature should be added in Eq. (21). However for simplified calculation, the present model is restricted to temperature as a constant or a linear relation to time. Then for the chain reaction HF chemical laser, the  $R_s(\nu)$  can be evaluated from Eq. (17) with just changing [HF] to  $\{[\text{HF1}] + [\text{HF2}]\}$  and adding one more term  $a_2(\nu)k_2[\text{H}][\text{F}_2]$  due to the reaction (R-2).

The total concentration of lasing species is given by

$$\sum_{\nu=0}^{\nu} n(\nu) = n_s = [\text{HF1}] + [\text{HF2}] \quad (23)$$

Since Eq. (11) is rewritten as,

$$n(\nu+1) = n(\nu) \exp(-2J\delta) \\ + \frac{a_s(\nu, J) \exp((J^* - J)\delta)}{J} \quad (24)$$

$n(\nu)$  can be expressed in terms of  $n_s$  as,

$$n(0) = \frac{1}{1-X^2} \{ (1-X) n_s - Y \{ U(0) (1-X^2) \\ + U(1) (1-X^2) + U(2) (1-X) \} \} \\ n(1) = \frac{1}{1-X^2} \{ X(1-X) n_s - Y \{ U(0) (X-1) \\ + U(1) X(1-X^2) + U(2) X(1-X) \} \} \\ n(2) = \frac{1}{1-X^2} \{ X^2(1-X) n_s - Y \{ U(0) X(X-1) \\ + U(1) (X^2-1) + U(2) X^2(1-X) \} \} \\ n(3) = \frac{1}{1-X^2} \{ X^3(1-X) n_s - Y \{ U(0) X^2 \\ (X-1) + U(1) X(X^2-1) + U(2) \\ (X^2-1) \} \} \quad (25)$$

where

$$X = \exp(-2J\delta)$$

$$Y = \exp((J^2 - J)\delta) / J$$

$$U(v) = \alpha_n(v, J) / \alpha_r(v), v=0, 1, 2$$

At constant temperature,  $dn(v)/dt$  is given simply by,

$$\frac{d}{dt} n(v) = \frac{X^v(1-X)}{1-X^4} \frac{d}{dt} n_4 \quad (26)$$

However when temperature is a function of time, all of the  $X, Y, U(v)$  become functions of time. Thus in this case, the time derivatives of Eq. (25) have to be evaluated newly.

Finally, during lasing,  $R(v)$  is evaluated from Eq. (15) and the output-power is calculated from Eq. (16) for the chain reaction system.

#### 4. RESULTS AND DISCUSSION

In the present calculation, following initial conditions are taken,

$$\rho = 9.4072 \times 10^{-7} \text{ mole/cm}^3$$

$$T_0 = 300 \text{ K}$$

$$p_t = 1.207 \text{ atm}$$

$$[F]_0 : [H_2]_0 : [F_2]_0 : [Ar] = 0.1 : 1 : 1 : 50$$

$$r = \sqrt{r_0 r_1} = 0.9$$

$$L = 100 \text{ cm}$$

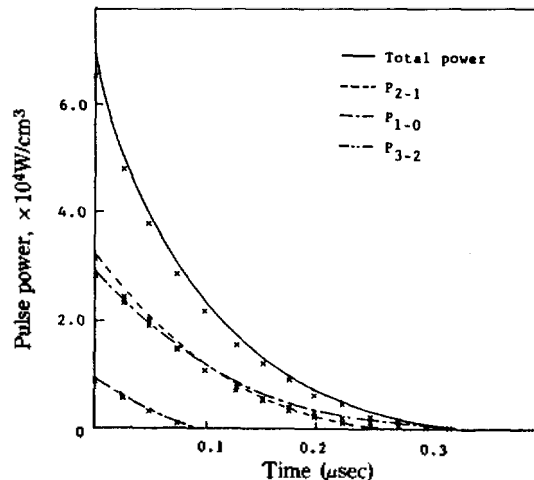


Fig. 1. Comparison between the anharmonic corrected and the harmonic approximated laser power in non-chain reaction: solid line-anharmonic corrected, x: harmonic approximated case.

Here,  $[F_2]_0$  is for the chain reaction system, and for the nonchain case, the inert diluent,  $[Ar]$  has to be added up for replacing  $[F_2]_0$ .

In the non-chain reaction  $F + H_2$  system, the kinetics is involved with (R-3), (R-4), (R-5) and (R-6) as well as (R-1) in Table 1. To verify differences of harmonicity from anharmonicity, the output-power from Eq. (1) and (11) are calculated separately and compared between them. As shown in Fig. 1, the difference is very small. For each level, the agreement is  $1 \rightarrow 0$  case is excellent, while for  $3 \rightarrow 2$  case, the agreement is good. As it was noted previously in section 2.2, this is an expected one. However, if the higher vibrational levels are included, the anharmonicity should be considered for a precise calculation. Thus in the present model with considering the lasing vibrational state up  $v = 3$ , the assumption of harmonicity would be quite reasonable. From this point, all of the calculations in the following will be performed with the harmonicity, by using Eq. (11) only.

Fig. 2 shows the  $H_2$ -concentration dependence to the laser power and duration time. As the initial concentration of  $H_2$  is increased, the peak power is increased and the duration time is decreased. It seems that as the  $H_2$  concentration increases, the consumption of F-atom is increased and

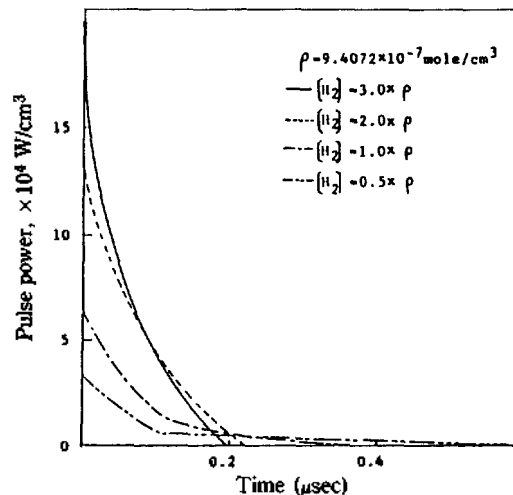


Fig. 2. Effect of the concentration of  $H_2$  on power vs. time in non-chain reaction.

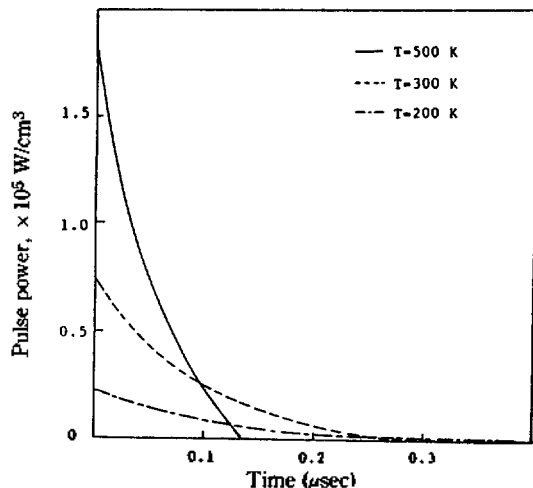


Fig. 3. Effect of temperature on power vs. time in non-chain reaction.

consequently disappearance time of the F is shortened. To find temperature dependence, the power calculations at  $T = 200, 300, 500$  K are shown in Fig. 3. In this figure, as the temperature is increased, the peak power is increased, while the duration time is decreased. Since rate constants are increased for temperature being increased, the production rate of HF is increased and disappearance of F-atom is fastened. This calculated resultant power of the non-chain system is similar to the experimental results<sup>18</sup> of  $SF_6$  chemical laser. When one compromise a variation of F-atom concentration due to a initiation mechanism, the present model would give good comparison with experimental data.

For the chain reaction system of  $H_2 + F_2$ , the chemical kinetics has involved all the reactions in Table 1. These 30 reactions are selected from the 68 reactions in the paper by Kerber *et al.*<sup>7</sup> And the vibrational levels are considered up to  $v = 6$  and are included up to  $v = 3$  for lasing species. The concentrations of important reactants, H, F,  $H_2$ ,  $F_2$ , and output-power are evaluated in terms of time propagation for  $T = 300$  K and  $T = a + bt$ .

For constant temperature, Fig. 4 are corresponded to the results for H and F-atom, and Fig. 5 for  $H_2$  and  $F_2$  molecules. The concentration of F-atom is decreased very sharply in the earlier

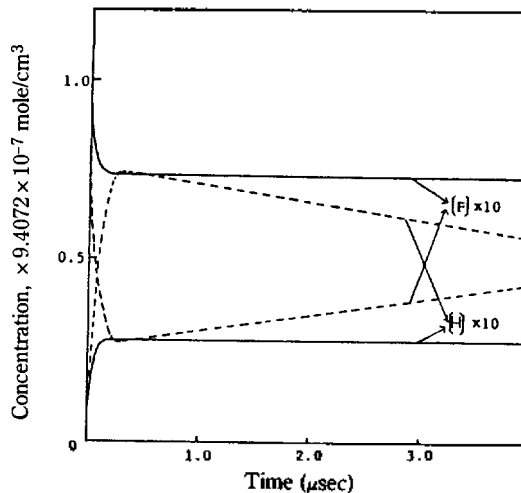


Fig. 4. The concentration of H, F vs. time in chain reaction. —  $T = 300$  K — —  $T = (300 + 1.5 \times 10^8 \cdot \text{time})$  K.

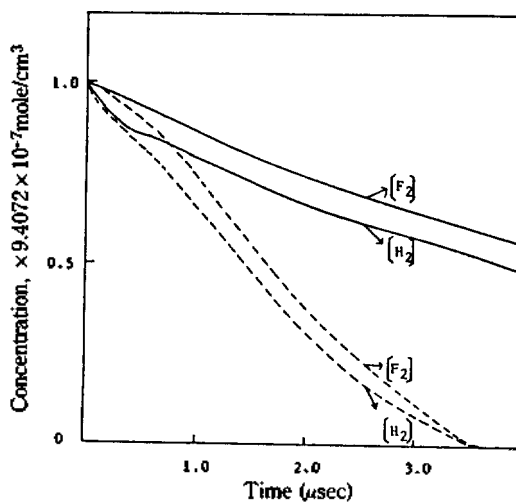


Fig. 5. The concentration of  $H_2$ ,  $F_2$  vs. time in chain reaction. —  $T = 300$  K, — —  $T = (300 + 1.5 \times 10^8 \cdot \text{time})$  K.

stage and after minimum point is increased very slowly, while the concentration of H-atom is increased very rapidly in the earlier stage, passed maximum point, and decreased very slowly. For  $H_2$  and  $F_2$  both molecules are consumed slowly. And that consumption of  $H_2$  is greater than  $F_2$  can be interpreted as reaction (R-I) *i.e.* (R-7), leads up (R-II) even though the reverse reaction of (R-I), for high vibrational HF recharges  $H_2$  concentration. The pulse power as shown in Fig. 6 displays that 2→1 transition is superior to 3→2 and 1→0 transitions. And when the total power in

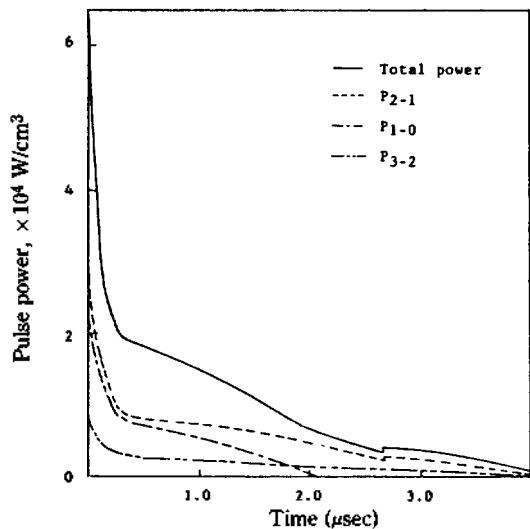


Fig. 6. Laser power for total and first three levels of HF vs. time for  $T = 300\text{K}$  in chain reaction.

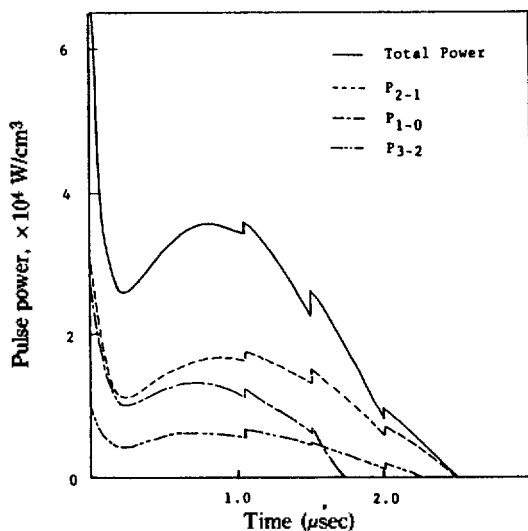


Fig. 7. Laser power for total and first three levels of HF vs. time for  $T = (300 + 1.5 \times 10^8 \cdot \text{time})\text{K}$  in chain reaction.

the chain reaction system is compared with that in the non-chain system through Fig. 6. and Fig. 3, one can see that even though the initial peak powers are almost same, the power of the chain system keeps on being generated up to  $4\mu\text{s}$ , while the power of the non-chain system is terminated within  $0.3\mu\text{s}$ .

To simplify the calculations, the temperature is assumed to be constant. However in a real system, the temperature is known to be increased slowly,

even though the increasing is repressed by inert diluents. Thus present model is attempted calculations with a simpler form of the temperature as  $T = a + bt$ . The constants  $a$  and  $b$  are taken arbitrary from the figure which was reported through detailed numerical simulation<sup>7</sup> by Kerber *et al.* The results from this temperature variation are plotted in Fig. 4, 5, and 7. In Fig. 4 the concentration of F in comparing with  $T = 300\text{K}$  case is decreasing much faster initially, reaches minimum at  $0.3\mu\text{s}$  and is increasing slowly up to half of initial concentration of F atom. The concentration of H atom is showing symmetrical behavior to the F atom. As shown in Fig. 5,  $\text{H}_2$  and  $\text{F}_2$  are consumed faster than the case of  $T = 300\text{K}$  and consumption rates are effectively constant. And the time history of the pulse power is decreasing rapidly up to  $0.3\mu\text{s}$  similar to the case of  $T = 300\text{K}$ , but after showing minimum point around  $0.3\mu\text{s}$  is increasing to maximum around  $0.8\mu\text{s}$  and then slowly decreasing to termination around  $2.5\mu\text{s}$ . This pulse power shows a good agreement with the result<sup>7</sup> calculated detailly by Kerber *et al.*

From this, the present model may give a confirmation that a very complicated calculation, which is included equations of states of all the involving species and conservations of mass, momentum and energy, can be replaced by a much simpler method. We believe that is characteristic parameters for a real system are considered, one can compare numerical calculations with experimental data.

#### ACKNOWLEDGEMENTS

This research was supported by the Korea Science and Engineering Roundation (KSEF).

#### REFERENCE

1. R. W. F. Gross and J. F. Bott (ED), "Handbook of Chemical lasers," John Willey & Sons, N.Y., 1976.
2. J. V. V. Kasper and G. C. Pimentel, *Phys. Rev. Lett.*, **14**, 352 (1965).
3. N. Cohen and T. A. Jacobs, *Int. J. Chem. Kinet.*, **1**,



- 495 (1969).
4. J. R. Airey, *J. Chem. Phys.*, **52**, 156 (1970).
  5. G. Emanuel, *J. Quant. Spectrosc. Radiat.*, **11**, 1481 (1971); "Analytical Model for a Continuous Chemical Laser," Tech. Rep. TR-0059 (The Aerospace Corp., Los Angeles, Cal. 1970).
  6. G. Emanuel, *Appl. Optics*, **11**, 2047 (1972).
  7. R. L. Kerber and G. Emanuel, *Appl. Optics*, **11**, 1112 (1972); "Resale - 1: A Chemical Laser Computer Programs," Tech. Rep. TR-0172 (0776)-1 (The Aerospace Corp. Los Angeles, Cal. 1972).
  8. G. Emanuel, "Numerical Modeling of Chemical Lasers," in Ref. 1, p. 469~548.
  9. R. L. Kerber, N. Chen, and G. Emanuel, *IEEE J. Quant. Electron*, **QE-9**, 94 (1973); R. L. Kerber, *Appl. Optics*, **12**, 1157 (1973).
  10. T. O. Poehler, F. C. Pirkle, Jr, and R. E. Walker, *IEEE J. Quant. Electron*, **QE-9**, 83 (1973).
  11. V. I. Igoshin, V. Yu. Nikitin, A. N. Oraevskii, and V. N. Tomashev, *Sov. J. Quant. Electron*, **10**, 828 (1980); **11**, 166 (1981).
  12. R. L. Tayler, P. F. Lewis, and J. Cronin, *J. Chem. Phys.*, **73**, 5 (1980).
  13. T. D. Dreiling, *J. Appl. Phys.*, **61**, 1688 (1987).
  14. E. U. Baikov, A. S. Bashkin, N. M. Gamzatov, A. N. Oraevskii, and O. E. Porodinkov, *Sov. J. Quant. Electron*, **14**, 1548 (1984).
  15. D. E. Mann, *J. Chem. Phys.*, **34**, 420 (1961).
  16. J. M. Herbelin and G. Emanuel, *J. Chem. Phys.*, **60**, 689 (1974).
  17. R. E. Meredith and F. G. Smith, *J. Quant. Spectrosc. Radiat. Transfer*, **13**, 89 (1973).
  18. J. L. Lyman, *Appl. Optics*, **12**, 2736 (1973).