A Model and Simulation of TEA-CO2 Laser in Consideration of H2O Molecule in Active Gas

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Abstract: We have developed an output power prediction method used in the design of the output power of a TEA-CO2 laser which uses carbon dioxide and nitrogen produced by industrial method. In this paper, we have commented a method of modeling the laser output power and the simulation method based on the 7- vibrational temperature model which has six vibrational temperatures including a vibrational temperature of H2O molecule and the peripheral temperature which was constant and finally proved the simulation result.

Keywords: vibrational temperature, influence of H2O molecule, energy exchange process

1. Introduction

It is the first and foremost task to simulate exactly the energy exchange process between the particles of the active gases in a TEA-CO2 laser for the purpose of increasing the output power and the efficiency. The more exact the output power model of a CO2 laser reflects the oscillatory motion, the stimulated radiation, the spontaneous radiation and the loss in the resonator, the closer the simulation result is to practical experimental result. [1 to 14] The 5- vibrational temperature model for the output model of a CO2 laser, which takes account of the CO molecule produced during gas discharge has been developed. [11 to 20] The relaxation rate from a level 100 to a level 000 of carbon dioxide through V-T process when ignoring the effect of H2O gas is over 200 times as great as that when not ignoring it. And the relaxation rate from a level 010 to a level 000 through V-T process by H2O molecules which play the role of collision molecules is 140 times as great as than by helium molecules. The relaxation rate by helium is 100 times and 20 times as great as nitrogen and carbon dioxide respectively. [1, 7] Hence, the effect of H2O molecules is much greater than that of helium or argon gas Consequently, we have predicted that the output power model of a TEA-CO2 laser would be more accurate if the oscillatory motion between CO2, N2, CO and H2O molecules was taken into account. In this paper, we have proposed the 6- oscillatory motion equation in consideration of the vibrational mode of H2O molecules and set up the simulation method of the output power of a laser.

This paper is composed of as follows. Section 2 introduces the oscillatory motion equation of energy exchange relation between main components and impurity ones of the working gas in a TEA-CO2 laser. Section 3 presents a method of modeling the output power of a laser in consideration of population inversion, stimulated radiation, spontaneous radiation and loss of resonator. Section 4 presents the simulation method of the output power model. Section 5 illustrates the result of accuracy verification. Section 6 summarizes our results and discusses further applications.

2. The Oscillatory Motion Equation of Active Gases

In order to set up the model of the output power of a laser it is essential to know the population inversion which has direct influence on the output power. And to find the population inversion, the energy exchange relation between activated molecules ought to be analyzed. Namely, the oscillatory motion equation corresponding to the kind of vibrations of the molecules must be set up. We have set up the oscillatory motion equation as follows.

The variation of an energy density $E_i$ accumulated in a symmetry mode of a CO2 molecule with time is related with the following expressions:

$$CO_2(100) + M_i \leftrightarrow CO_2(000) + M_i$$

$$CO_2(100) + M_i \leftrightarrow CO_2(020) + M_i$$

$$CO_2(001) + M_i \leftrightarrow CO_2(110) + M$$

$$CO(1) + CO_2(000) \leftrightarrow CO_2(110) + CO(0)$$

$$CO_2(000) + e \rightarrow CO_2(100) + e$$

where $M_i$ means the kind of molecules (such as CO2, N2, H2, H2O, CO and O2 molecules) colliding with a level 100 of CO2 molecules.

The variation of $E_i$ with time is also made when a CO2 molecule transfers from a level 001 to a level 100 while emitting a photon of a wavelength 10.6 micrometer). In this case, the energy increase of the symmetric mode is written as $v_i \Delta N_{31} W_{v_i} (t)$, where $\Delta N_{31}$ is the difference of the population between the two levels, $I_{v_i}$ the light intensity in the center frequency and W is given as

$$W = \frac{\lambda_i^2 g(v)}{8 \pi v_i \tau_{\text{self}}}$$

where $\lambda_i$ is the wavelength corresponding to $hv_i$, $g(v)$ the normalized spectral function, $\tau_{\text{self}}$ the lifetime of spontaneous radiation.

Eventually, the oscillatory motion equation of the symmetric model is as follows [5, 6 and 20]:

$$\frac{dE_i}{dt} = \frac{E_i - E_i(T)}{\tau_a(T)} - \frac{E_i - E_i(T, T_1)}{\tau_1(T, T_1)} - \frac{hv_i}{\tau_2(T)} + \frac{hv_i}{\tau_{12}(T)} + \frac{hv_i}{\tau_{10}(T, T_1)} + \frac{hv_i}{\tau_{20}(T, T_1)} + \frac{hv_i}{\tau_{12}(T)} + \frac{hv_i}{\tau_{10}(T, T_1)} + \frac{hv_i}{\tau_{20}(T, T_1)} + \frac{hv_i}{\tau_{12}(T)} + \frac{hv_i}{\tau_{10}(T, T_1)} + \frac{hv_i}{\tau_{20}(T, T_1)} + \frac{hv_i}{\tau_{12}(T)} + \frac{hv_i}{\tau_{10}(T, T_1)} + \frac{hv_i}{\tau_{20}(T, T_1)}$$

where the suffixes 0, 1, 2 and 3 mean the ground state, the symmetric state, the deformation state, the asymmetric state of a CO2 molecule respectively, and 4, 5 and 6 does the vibrational states of N2, CO and a level 010 of H2O molecules, respectively.
And $\tau_{\text{async}}$, $\tau_{2\text{async}}$, $\tau_0(T, T_1)$, $\tau_{\text{sync}}(T, T_1, T_2)$, $\tau_{\text{sync}}(T, T_1, T_2, T_3, T_4)$, $E_1(T, T_1)$, $E_2(T, T_1)$, $E_3(T, T_1)$, $E_4(T, T_1)$, and $P_{\text{ext}}$ are written as

$$\tau_{\text{sync}}(T, T_1) = \tau_{\text{sync}}^{\text{1-x}}(T_1) - \tau_{\text{sync}}^{\text{1-x}}(T) = \sum N_x \chi^{\text{1-x}}_{\text{1-x}} \left( 1 - \exp \left( -\frac{hv}{kT} \right) \right)^{-1}$$

$$\tau_{\text{sync}}(T, T_1, T_2) = \tau_{\text{sync}}^{\text{1-x}}(T_1, T_2) - \tau_{\text{sync}}^{\text{1-x}}(T_1) - \tau_{\text{sync}}^{\text{1-x}}(T) = \sum N_x \chi^{\text{1-x}}_{\text{1-x}} \left( 1 - \exp \left( -\frac{hv}{kT} \right) \right)^{-1} \times \left( \exp \left( \frac{hv}{kT_1} \right) \right) \left( \exp \left( \frac{hv}{kT_2} - \frac{hv}{kT_1} \right) \right) \left( \exp \left( -\frac{hv}{kT} \right) \right)$$

$$\tau_{\text{sync}}(T, T_1, T_2, T_3, T_4) = \tau_{\text{sync}}^{\text{1-x}}(T_1, T_2, T_3, T_4) - \tau_{\text{sync}}^{\text{1-x}}(T_1, T_2) - \tau_{\text{sync}}^{\text{1-x}}(T_1, T_3) - \tau_{\text{sync}}^{\text{1-x}}(T_1, T_4) - \tau_{\text{sync}}^{\text{1-x}}(T_1) - \tau_{\text{sync}}^{\text{1-x}}(T) = \sum N_x \chi^{\text{1-x}}_{\text{1-x}} \left( 1 - \exp \left( -\frac{hv}{kT} \right) \right)^{-1} \times \left( \exp \left( \frac{hv}{kT_1} \right) \right) \left( \exp \left( \frac{hv}{kT_2} \right) \right) \left( \exp \left( \frac{hv}{kT_3} \right) \right) \left( \exp \left( -\frac{hv}{kT} \right) \right)$$

$$E_1(T, T_1) = \frac{\text{coefficient of travel rate, \text{volume in unit time, n, where}}}{N_{\text{CO}} \chi(T) = \exp \left( \frac{hv}{kT} \right) \left( \frac{h}{v} \right)}$$

$$E_1(T, T_1) = \frac{\text{coefficient of travel rate, \text{volume in unit time, n, where}}}{N_{\text{CO}} \chi(T) = \exp \left( \frac{hv}{kT} \right) \left( \frac{h}{v} \right)}$$

And the equation for a level 01/00 which is the deformation mode of a H₂O molecule is written as

$$\frac{dE_{\text{d}}}{dt} = P_{\text{ext}} \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T)$$

$$\left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T) \left( \frac{hv}{v_T} \right) E_{\text{d}} - E_{\text{d}}(T)$$

Where the terms in the right side mean the energy exchange relation in the following processes and H₂O molecules play the same role as helium and argon.

$$\text{H}_2\text{O}(000) \quad \text{+ e} \rightarrow 2 \text{H}_2\text{O}(010) + \text{e}$$

$$\text{H}_2\text{O}(000) + \text{CO}_2(100) \leftrightarrow \text{H}_2\text{O}(010) + \text{CO}_2(000) \text{H}_2\text{O}(000) + \text{CO}_2(020) \leftrightarrow \text{H}_2\text{O}(010) + \text{CO}_2(000) \text{H}_2\text{O}(010) + \text{M} \leftrightarrow \text{H}_2\text{O}(000) + \text{M}$$

The equations (1 to 6) are the basis of modeling of the output power model of a laser.

### 3. Output Power Model of Laser Authors

The output power directly is related with the population inversion. The population inversion \( \Delta N \) is written as [15, 16 and 20]

$$\Delta N = N_{\text{exc}} \cdot P(J) - N_{\text{rel}} \cdot P(J + 1)$$

$$N_{\text{exc}} = N_{\text{CO}} \exp \left( \frac{hv}{kT} \right) \left( \frac{h}{v} \right)$$

$$P(J) = \frac{B(J + 1)}{kT} \left( \frac{h}{v} \right)$$

where B is the rotation constant of a CO₂ molecule, c the velocity of light and Q is the degeneracy of a rotation state. Then, we should find the relation between the population inversion and the light intensity in the resonator. As it is, the increase of radiation density by stimulated radiation per unit time is written as [2]

$$\frac{h v c^3 \Delta (v) g(v) d v}{8 \pi h v^3 r_{\text{eff}}} = \frac{h v c^2 \Delta N I(v) \delta(v - v_0) g(v) d v}{8 \pi h v^3 r_{\text{eff}}}$$

From this, the increase velocity of the light intensity is written as follows

$$\frac{d I_{\text{m}}}{d t} = \Delta N c I_{\text{m}} g(v_0) \frac{1}{8 \pi v_0 r_{\text{eff}}}$$

where \( v_0 \) is the center frequency in the spectral function. Meanwhile, all losses in the mirrors can be specified by a single parameter \( r_{\text{res}} \) which is the lifetime of the resonator, and therefore we can write as follows

$$\frac{d I_{\text{m}}}{d t} = \frac{I_{\text{m}}}{r_{\text{res}}}$$

The minimum threshold of the population inversion is given at the maximum value of the spectral function \( g(v_0) \).

So the temporal change of the light intensity in the resonator is as follows [6]:

$$\frac{d I_{\text{m}}}{d t} = \frac{-I_{\text{m}}}{r_{\text{res}}} + \frac{c^3 \Delta N I_{\text{m}}}{4 \pi v_0^3 r_{\text{eff}}} = \frac{-I_{\text{m}}}{r_{\text{res}}} + \frac{c^3 \Delta N I_{\text{m}}}{4 \pi v_0^3 r_{\text{eff}}}$$

Now the spontaneous radiation ought to be taken into
account. From the general relation between stimulated radiation and spontaneous radiation, the term related to spontaneous radiation is written as [3]
\[ chvN_{0,01}P(J)/\tau_{self} = G \]
where G is the portion of the photons emitted spontaneously. Because these photons emit at a stereotype angle \( \beta \) which corresponds to the spread angle of the laser beam, the remainder in the resonator does at a certain angle with the optical axis of the resonator which is \( \beta/4\pi \). The spectral width \( dv \) of such photons is close to the center of the rotation transition line.

The portion of the radiation energy portion whose center value is \( v_0 \) and spectral width is \( dv \) is written as
\[ g(v_0)dv = \frac{2dv}{\pi\Delta v} \]
In our case the magnitude of \( \Delta v \) is more important than its detailed expression. In the standard condition, it is as follows [5]
\[ \Delta v \sim 4\text{GHz}, \quad dv \sim (2\pi\tau_v)^{-1} \]
Hence,
\[ G = \frac{\beta}{4\pi} \frac{2dv}{\pi\Delta v} \]
Then, the term related to the spontaneous radiation is as follows
\[ chv_0N_{0,01}P(J)\beta dv = \frac{2\pi^2\tau_{self}\Delta v}{2\pi^2\tau_{self}\Delta v} \]
Therefore, the light intensity in the resonator is determined by the following equation
\[ \frac{dI_\text{res}}{dt} = \frac{I_\text{res}}{\tau_{res}} + \frac{\Delta NWI_{res} + N_{0,01}P(J)S}{h} \] (8)
where
\[ S = \frac{\beta dv}{2\pi^2\tau_{self}\Delta v} \]
In order to apply Eq.8 in the calculation of the laser output, it is necessary to find the detailed expression of \( \tau_{res} \).

Assume that there is a stable resonator of a length \( L \), the optic axis coincide with \( z \) axis, which is filled up with homogeneous active material of a gain through a length \( \ell \).

In this case the following relation comes into being.
\[ \alpha = -\left(1/2\ell\right)\ln[R(1 - \delta)] \] (9)
where R is the reflectivity of the output mirror and \( \delta \) the sum of all the losses in the output mirror.

Finally, the output power of the laser can be expressed as follows
\[ P_{\text{out}} = A(1 - R - \delta + \delta R)I_0 \] (10)
where \( A \) is the area of the cross section of the output mirror and \( I_0 \) the light intensity in it. It is impossible to calculate the flux density of radiation energy \( I(z) \) in static method but it’s possible to do the average light intensity. i.e.
\[ \langle I_\text{res} \rangle = \frac{1}{\ell} \int_0^\ell I(z)dz = \frac{1}{\ell} \int_0^\ell (1 - \delta)RI_v(e^{j\alpha} + e^{j(2\ell - 1)})dz = \]
\[ = -\frac{(1 - \delta)RI_v}{\alpha\ell} + \frac{(1 - \delta)RI_v e^{2\alpha\ell}}{\alpha\ell} \]
Considering Eq.8, we obtain
\[ \langle I_\text{res} \rangle = -\frac{2[1 - R(1 - \delta)]}{\ln[R(1 - \delta)]]} I_v \] (11)
and substituting \( I_0 \) into eq.10
\[ P_{\text{out}} = \frac{A}{2}\ln[R(1 - \delta)]I_v \frac{1 - R - \delta + \delta R}{1 - R(1 - \delta)} \]
The above-mentioned method is one of calculating the laser output power.

Now, the magnitude of \( \tau_{res} \) in eq.8 is calculated as follows. The sum of losses such as diffraction loss and the other ones in eq.12 is the same as
\[ P_{\text{out}} = \frac{A}{2}\ln[R(1 - \delta)]I_v \frac{1 - R - \delta + \delta R}{1 - R(1 - \delta)} \]
Therefore, the rate of the variation of the light intensity in the output mirror due to the effective loss and the ineffective ones is written as
\[ \left( \frac{d(I_{\text{res}})}{dt} \right)_{\text{loss}} = \frac{P_{\text{out}} + P_{\text{loss}}}{A\ell} - C = \frac{C}{\ell} \left(1 - R + \delta R\right)I_v = \frac{\langle I_{\text{res}} \rangle}{\tau_{\text{res}}} \]
Hence, \( \tau_{res} \) is
\[ \tau_{res} = -\frac{2I_v}{C\ln[R(1 - \delta)]} \] (13)

4. Simulation of Laser Output Power

The simulation is composed of three steps: initialization of input parameters, solving, and optimization. In the first step, we input the reference data for the calculation of the output power.

Next, we get the vibrational temperatures \( T_i (i=1 \text{ to } 6) \). [20]
\[ T_i = \frac{h}{k} \ln(1 + N_i h v_i / E_i) \]
where \( i=1 \text{ to } 6 \) correspond to the vibrational modes of the CO2, N2 and H2O molecules. And we calculate from eq.7 to eq.13.

In this case the initial conditions is as follows
\[ E_1(0) = (1 - f)N_{CO2}hv_1 / (exp(hv_1 / kT) - 1) \]
\[ E_2(0) = (1 - f)N_{CO2}hv_2 / (exp(hv_2 / kT) - 1) \]
\[ E_3(0) = (1 - f)N_{CO2}hv_3 / (exp(hv_3 / kT) - 1) \]
\[ E_4(0) = N_{N_2}hv_4 / (exp(hv_4 / kT) - 1) \]
\[ E_5(0) = (fN_{CO2} + N_{CO})hv_5 / (exp(hv_5 / kT) - 1) \]
\[ E_6(0) = (N_{H_2O}hv_6 / (exp(hv_6 / kT) - 1) \]
\[ E(0) = 0, \quad T = 300K, \quad I_v(0) = 1E - 9 \]
Because of the good cooling condition, the value of T is constant.

Table.1 shows the coefficients and the constants used in the calculation. [1 to 15]
We used the result of [4 and 7] as an electron density Ne(t). Fig.1 shows the calculation result of the output power related to the amount of H2O. In fig.1, the curves from 1 to 5 correspond to the cases CO2: N2: H2O = 1:9:0.02, CO2: N2: H2O = 1:9:0.08, CO2: N2: H2O = 1:9:0.14, CO2: N2: H2O = 1:9:0.2, CO2: N2: H2O = 1:9:0.26, respectively. From the fig.1 it is noted that the output power increases and then decreases while increasing the amount of H2O. This means that there is an optimal value in the amount of H2O and it is the same as CO2: N2: H2O = 1:9:0.2.

With the experimental ones in [15] which is shown in Tab.2.

Fig.2 shows the simulation result of the laser output power and fig.3 the experimental result in [15].

In comparison of fig.2 with fig.3, it is clear that the simulation result is so close to the experimental one for the maximum pulse power and the pulse width. And the trend of the simulation result is similar to that in [20].

Consequently, it is available to design a high-power TEA-CO2 laser using the model of calculating the output power and the code. In other words, the model and the simulation method helps to predict the energy of laser pulse, the peak power, the average power, the pattern of the pulse, the composition ratio, the total pressure, the effective loss and ineffective losses and get the optimal basic parameters of a TEA-CO2 laser demanded for the desired output power.

5. Verification of Simulation of Laser Output Power

We compared the simulation result with the experimental one showed in [15]. In the simulation, the initial data coincide with the experimental ones in [15] which is shown in Tab.2.

### Table 2: Experimental data in [15]

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<th>Parameter</th>
<th>Comment</th>
<th>Value</th>
<th>Unit</th>
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<tr>
<td>$X_1$</td>
<td>Coefficient of excitation velocity(CO$_2$ (100))</td>
<td>5.0×10$^{-10}$</td>
<td>cm$^3$/s</td>
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<tr>
<td>$X_2$</td>
<td>Coefficient of excitation velocity (CO$_2$ (010))</td>
<td>3.0×10$^{-9}$</td>
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<td>Coefficient of excitation velocity (CO$_2$ (001))</td>
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<td>Coefficient of excitation velocity (N$_2$ (v=1))</td>
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<tr>
<td>$X_5$</td>
<td>Coefficient of excitation velocity (CO (v=1))</td>
<td>3.0×10$^{-8}$</td>
<td>cm$^3$/s</td>
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<tr>
<td>$J$</td>
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<td>-</td>
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<tr>
<td>$L$</td>
<td>Length of resonator</td>
<td>120</td>
<td>cm</td>
</tr>
<tr>
<td>$e$</td>
<td>Length of active material</td>
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<td>cm</td>
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<td>Reflection coefficient of output mirror</td>
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<tr>
<td>$\delta$</td>
<td>Loss coefficient of resonator</td>
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<td>$f$</td>
<td>Degree of dissociation of CO$_2$ molecule</td>
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<td>$A$</td>
<td>Area of output mirror</td>
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<td>Cm$^2$</td>
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<td>$\text{CO}_2$:$\text{N}_2$:$\text{H}_2$O</td>
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<td>1:1:8</td>
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<td>He</td>
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### Table 1: Coefficients and constants

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<td>$h\nu_1$</td>
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<td>6.625×10$^{-3}$ erg/s</td>
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<tr>
<td>$h\nu_2$</td>
<td>667 cm$^{-1}$</td>
<td>$J$</td>
<td>18</td>
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<td>$h\nu_3$</td>
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<td>$p$</td>
<td>760 Torr</td>
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<td>$X'_2$</td>
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<td>$B_{CO_2}$</td>
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<td>$R$</td>
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<td>$X'_4$</td>
<td>2.3×10 cm/s</td>
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<td>$X'_5$</td>
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<td>CO$_2$:N$_2$:H$_2$O</td>
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<tr>
<td>$X'_6$</td>
<td>5×10$^{-8}$ cm/s</td>
<td>$f$</td>
<td>0.2</td>
</tr>
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### Figure 1: Calculation result of the output power corresponding to the amount of H2O (1-CO2:N2:H2O = 1:9:0.02, 2-CO2:N2:H2O = 1:9:0.08, 3-CO2:N2:H2O = 1:9:0.14, 4-CO2:N2:H2O = 1:9:0.2, 5-CO2:N2:H2O = 1:9:0.26).

### Figure 2: Simulation result
6. Conclusion

In this paper, we have developed an available model of the output power of a TEA-CO₂ laser which uses carbon dioxide and nitrogen produced by industrial method. Through the simulation, it was verified that the result from this model coincided approximately with the experimental result. The developed model and simulation method can be used for designing the main generator and the amplifier of a TEA-CO₂ laser using carbon dioxide and nitrogen produced by industrial method.

7. Acknowledgment

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References