Numerical Simulation of Throat-mixing System for Supersonic Flow Chemical Oxygen-Iodine Laser*

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Throat-mixing systems are proposed and assessed for the supersonic flow chemical oxygen-iodine laser (S-COIL). Three-dimensional, numerical simulation solving the governing equations of compressible gas flows together with chemical kinetics has been made for investigating the characteristics of the mixing condition and chemical reactions. The compressible Navier-Stokes equations and a chemical kinetic model encompassing 21 chemical reactions and 10 chemical species are solved by means of a full-implicit finite difference method. Two types of nozzles, a blade- and cylinder-type nozzles are adopted. The results show satisfactorily high values of the small signal gain coefficient $G$. The proposed throat-mixing system shows higher efficiency than the parallel mixing system. The blade-type nozzle is found to give 44% higher peak value of $G$ than that of the parallel mixing system. It is also noted that the cylinder-type nozzle has superior ability than the parallel mixing system, in spite of its exceedingly simple structure.

Key Words: Supersonic Flow, Laser, Numerical Analysis, Throat Mixing, Oxygen, Iodine

1. Introduction

Supersonic flow chemical oxygen-iodine laser (S-COIL) has attracted substantial interests in recent years\cite{10,11}, since it is supposed to improve the efficiency and laser power of chemical oxygen-iodine laser (COIL) by gas cooling via supersonic expansion.

The principle of the COIL is based on the energy transfer from the excited oxygen molecule to the iodine atom and the light emission from the excited iodine atom. Those reactions can be expressed as follows:

\begin{align}
O_2(\Delta) + I(2P_{3/2}) & \rightarrow O_2(\Sigma) + I(2P_{1/2}), \\
I(2P_{1/2}) & \rightarrow I(2P_{3/2}) + h\nu,
\end{align}

where $O_2(\Delta)$, $O_2(\Sigma)$, $I(2P_{3/2})$, $I(2P_{1/2})$, and $h\nu$ are the oxygen molecule in the excited state, that in the ground state, the iodine atom in the ground state, that in the excited state, and the emitted photon, respectively. In reality, the overall reactions shown above consist of numerous elementary reactions, which includes $I(2P_{1/2})$ consumption without contributing to the emission of laser light. It has been found that the balance of the rates of gas mixing and chemical reactions is of significant importance for the performance of the laser\cite{10,11}. If the iodine gas is injected into the gas flow of $O_2(\Delta)$ at subsonic region upstream the throat of the expansion nozzle, mixing and chemical reactions may occur too quickly so that the gas in the resonating region located downstream of the flow no longer contains sufficient amount of $I(2P_{1/2})$. On the other hand, if the iodine gas is introduced in the supersonic flow region downstream the nozzle, the mixing rate of the reacting gas species would be slow since the flow becomes laminar, and dominates the reaction (1), accordingly.

In the previous study\cite{10}, a parallel mixing system, in which iodine gas is introduced in the supersonic
flow region, was found to give good performance if ramp nozzle arrays are adopted and strong vortices are given in the flow. However, this system needs complex nozzle arrays. In the practical point of view, simple nozzle is desirable. A throat-mixing system, in which the iodine gas is introduced into the \( O_2(A) \) flow at the throat of the expansion nozzle, is expected to enhance the mixing performance with relatively simple nozzle-shape compared to the parallel mixing system since the mixing takes place upstream the developed supersonic-flow. Thus, in this study, throat-mixing systems for the S-COLL are examined adopting two types of simple nozzles, a blade-type nozzle and cylinder-type nozzle.

![Diagram of nozzle geometries and calculating domains](image)

(a) Parallel mixing system (Ramp nozzle)

(b) Throat-mixing system (Blade-type nozzle)

(c) Throat-mixing system (Cylinder-type nozzle)

Fig. 1 The nozzle geometries and the calculating domains

2. Mathematical Modeling and Numerical Methods

2.1 Configuration of flow field

In order to assess the effectiveness of the laser power, parallel mixing and throat-mixing systems are computed. Figure 1 shows the nozzle geometries and calculating domains. The parallel mixing system (Fig. 1(a)) has an array of ramp nozzles of \( O_2 \) and \( I_2 \) in an alternating arrangement. The \( O_2 \) and \( I_2 \) gases are introduced to each of the nozzles at the upstream and expanded separately to the downstream supersonic condition. Downstream of the base relief region, these two streams join in parallel. The mixing and reaction are significantly accelerated by the strong streamwise vortices produced by the ramp nozzle array, as it has been shown in the previous paper\(^a\). The geometry and boundary condition of the system are essentially the same to those adopted in the previous work. However, it is calculated again since the revised chemical model\(^b\) is adopted in this study.

The throat-mixing system, on the other hand, has nozzles composed of an array of blades (Fig. 1(b)) or cylinders (Fig. 1(c)). Each blade or cylinder has rows of orifices of 0.5 mm in diameter on both sides in order to inject the \( I_2 \) gas into the primary flow of \( O_2 \) gas at the nozzle throat.

It is assumed that all of the \( I_2 \) jets have the same shape and that each jet has a symmetric plane that parts the orifice in the center. The computational domain indicated by the broken lines in Fig. 1 is used in the present calculation. The \( x \)-axis in the parallel mixing system is a coordinate parallel to the primary flow with its origin at the nozzle exit plane, and that in the throat-mixing system is the one with its origin at the center of the \( I_2 \) injecting orifices. The \( y \) and \( z \)-axes are coordinates perpendicular to the \( x \)-axis.

2.2 Mathematical modeling

The model and method used here are essentially the same as those in the previous papers\(^a,b\). The laser emission is not considered. The governing equations, i.e., the three-dimensional full Navier-Stokes equations, in the physical domain are transformed to the computational domain and discretized using the cell-centered finite volume method. The higher-order Roe's flux difference splitting scheme with the monotone upstream-centered schemes for conservation laws (MUSCL) approach and the van Albada's limiter are applied for space discretization of the convection terms, and the central difference scheme for viscous terms. The steady-state solution is obtained using the lower-upper symmetric Gauss-Seidel (LU-SGS) method with local time steps for time integration of the governing equations. The domains are divided
into several blocks, each of which has calculating cells constructed according to the body-fitted coordinates. The domain includes 231,900 cells for the parallel mixing system adopting ramp nozzle (Fig. 1 (a)), 81,600 cells for the throat-mixing system adopting blade-type nozzle (Fig. 1 (b)), and 70,125 cells for the throat-mixing system adopting cylinder-type nozzle (Fig. 1 (c)).

In the present calculation, a chemical kinetic model proposed by Madden, Hager, Lampson, and Crowell(13) is used for the evaluation of the chemical composition of the mixture. Table 1 shows the model, which consists of 10 chemical species and 21 chemical reactions. This model is newer than the one that had been adopted in the previous work(19) where the numerical result of the parallel mixing system is shown. Thus, the calculation for this system is made again in this work. Catalytic reactions on the wall and water condensation are neglected.

The wall boundary conditions are isothermal, non-slip and non-catalytic, while the mirror reflection rule is applied on the symmetric boundaries. At the upstream boundary of the O2 and I2 flow, the plenum pressure, total enthalpy and molar fractions are imposed, and the velocity, which is assumed to be parallel to the x-axis, is obtained using a simple linear extrapolation from the interior cells. The sonic condition for the I2 flow is further imposed at the orifices for the throat-mixing systems. At the downstream boundary, all variables are calculated using zero gradient conditions.

The plenum conditions of the primary flow from the chemical oxygen generator and the secondary flow of I2 gas are shown in Table 2. Equivalent conditions except pressure are applied for parallel mixing and throat-mixing systems. The pressures of the primary and secondary flows are varied in order to adjust mixing condition of the flows for each system. The initial excitation efficiency of oxygen is defined as

\[ \eta = X_0[O_2(\Delta)]/X_{0}[O_2(\text{total})], \]

where \( X \) is the mol fraction and the subscript 0 indicates the initial condition. It is seen from Table 2 that \( \eta = 0.5 \) is assumed in the present calculation.

3. Results and Discussion

3.1 Flow and mixing

Figure 2 (a) shows the streamlines, for the parallel mixing system, issuing from the downstream corners of the nozzle and the intersections of the surfaces.
consisting of the streamlines with the $y$-$z$ planes. It is seen that a streamwise vortex is induced downstream of the base relief region. The extent of the vortex especially grows in the region of $0 \leq x \leq 70$ mm. In the downstream region of $x > 70$ mm, the growth of the extent of the vortex is insignificant. It is noted that the enhancement of the mixing due to the vortex in the downstream region is only around the center of the vortex.

Figures 2(b) and (c) show the streamlines and the cross sections of the stream tubes of the $I_2$ jets issuing from the circular orifices for the blade-type and cylinder-type nozzles, respectively. The thick line in each figure is defined as the streamline issuing from the orifice center. Although the $I_2$ jet injected from the orifice deviates rapidly from the injected direction due to the strong shear force, it seems to penetrate sufficiently into the primary flow and spreads widely in the domain. The penetration and the properties of a jet injected transversely into a primary flow depend mainly on the effective velocity ratio $\Gamma$, which is defined as the square root of the ratio of the momentum flux across the jet orifice to that of the primary flow, namely,

$$\Gamma = \sqrt{\frac{\rho_0 U_2^2}{\rho U^2}},$$

where $\rho$ and $U$ denotes density and velocity, and subscripts $p$ and $s$ represent primary and secondary flows, respectively. In the present calculation, the values evaluated from the numerical results are $\Gamma = 2.51$ for the blade-type nozzle and 2.79 for the cylinder-type. These values of $\Gamma$ seem to be appropriate from the viewpoint of mixing, since the stream tubes of the injected jets expand widely in the domain. It should be noted that the streamwise vortexes induced by the injection of the secondary jets stretch the stream tube in $y$- and $z$-direction downstream from the orifice.

Though the cylinder-type nozzle causes similar flow behavior (Fig.2(c)) to that of blade-type (Fig.2(b)), the extent of the vortex seems to be narrower than that in the case of blade-type nozzle. It is plausible to interpret that the vortex in the cylinder-type nozzle expands narrower area than that in the blade-type, since the cylinder-type nozzle has shorter path length, only 4.3 mm, for the supersonic expansion than 20 mm in the path length of the blade-type nozzle.

3.2 Distribution of the small signal gain coefficient

Small signal gain coefficient $G$ is regarded as an index of the efficiency of the laser, and is calculated from the following equation:

$$G = \frac{7}{12} \left[ \ln \frac{2}{\pi} \frac{A \lambda^2}{4 \pi} \frac{K(\phi)}{\Delta v_p} \right] [I(P_{12})]$$

Fig. 3 Distribution of the small signal gain coefficient $G$ in the flow fields. (a) Parallel mixing system (ramp nozzle), (b) Throat-mixing system (blade-type nozzle), (c) Throat-mixing system (cylinder-type nozzle)

$$K(\phi) = \exp(\phi^3) \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^\infty \exp(-t^2) dt \right],$$

$$\phi = \sqrt{\ln \frac{2}{\pi}} \frac{A \lambda^2}{\Delta v_p}$$

where $A$ denotes the Einstein coefficient, $\Delta v_p$ the Doppler broadening, $\Delta v_c$ the pressure broadening, $n$ the number density of each species and $g$ the degeneracy of each species. Higher density of $I(P_{12})$ and lower density of $I(P_{33})$ give higher value of $G$. The laser cavity should be placed at the position where $G$ reaches to the highest, in order to achieve the highest efficiency. Thus, the distribution of $G$ along the $x$-direction is of essential concern. Since the small signal gain coefficient $G(x, y, z)$ is distributed in the three-dimensional domain, the average $G(x)$ of small signal gain coefficient in the $y$-$z$ plane is evaluated as follows:

$$G(x) = \frac{1}{S} \iiint Gdydz,$$

where $S$ is the area of the flow region on the $y$-$z$ plane at the location of $x$.

Figure 3(a) shows the three-dimensional distribution of the small signal gain coefficient $G$ in the flow.
field of the parallel mixing system. In the upstream, $G$ increases around the contacting surface of the two streams of $O_2$ and $I_2$, especially around the center of the streamwise vortex, as shown in the cross-sectional profile at $x=28$ mm. However, $G$ around the center of the vortex decreases as the gas flows to the downstream. It is seen that nearly 1/3 of the area of the cross-section of $y$-$z$ plane is occupied by negative value of $G$ throughout the flow field.

Figures 3(b) and (c) show the distributions of $G$ in the flow fields of the throat-mixing systems adopting blade- and cylinder-type nozzles, respectively. In the system adopting blade-type nozzle (Fig. 3(b)), $G$ increases and reaches to significantly high value in the central region of the $y$-$z$ plane as shown in the cross-section at $x=37$ mm. Although the high value region of $G$ vanishes as the gas flows to the downstream, almost entire area of the cross-section of $y$-$z$ plane is occupied by positive value of $G$. Similar tendency is seen in the system adopting cylinder-type nozzle (Fig. 3(c)).

Figure 4 shows the distribution of $G$ along the $x$ direction. It is seen that $G$ for the parallel mixing system starts to increase at $x=15$ mm, reaches to the maximum $G=0.5$ m$^{-1}$ at $x=68$ mm, and then slightly decreases with periodic fluctuation. The fluctuation in $G$ is seen both for the parallel mixing and for the throat-mixing systems. It is plausible that this fluctuation is caused by pressure waves stabilized in a supersonic-flow field. For the throat-mixing systems, on the other hand, $G$ steeply increases after the flow has passed through the nozzle. The maximum values of $G$ for the blade- and cylinder-type nozzles are, 0.72 m$^{-1}$ at $x=47$ mm, and 0.63 m$^{-1}$ at $x=25$ mm, respectively. The results show that the throat-mixing system obeying blade-type nozzle has the peak value 44% higher than that of parallel mixing system. It should be noted that even the cylinder-type nozzle gives 26% higher peak value in spite of its remarkably simple structure. Though the efficiency of the cylinder-type nozzle is less than the blade-type nozzle, it still has superior ability than the parallel mixing system. Since this nozzle has great advantage in its exceedingly simple structure, it is one of the most promising systems in a practical use.

4. Conclusions

Throat-mixing systems for the supersonic flow chemical oxygen-iodine laser (S-COIL) are investigated by computing three-dimensional, numerical simulation. Two types of nozzles are adopted, namely, blade- and cylinder-type nozzles. In comparison with a parallel mixing system adopting ramp nozzle array, which has shown good performance in the previous study, the throat-mixing systems are found to give better performance. The results show that the average small signal gain coefficient $G$ for the throat-mixing system increases in shorter distance of $x$ compared to that of parallel mixing system. The blade-type nozzle gives the highest peak value of $G=0.72$ m$^{-1}$, which is 44% higher than that of ramp nozzle adopted in the parallel mixing system. The cylinder-type gives the peak value of $G=0.63$ m$^{-1}$ and this is still 26% higher than the ramp nozzle. In both the throat-mixing systems, the stream of the secondary flow injected from the orifice at the throat of the nozzle spreads widely in the domain compared to that in the parallel mixing system. The superior performance of the throat-mixing system is supposed to arise from these mixing conditions. It is concluded that the throat-mixing system, especially the system adopting cylinder-type nozzle, are found to give more than competitive performance than the parallel mixing system even though it has great advantage in its exceedingly simple structure.

References


