Three-Dimensional Mixing/Reacting Zone Structure in a Supersonic Flow Chemical Oxygen-Iodine Laser*

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The flow field of a supersonic flow chemical oxygen-iodine laser is simulated by solving three-dimensional Navier-Stokes equations and the effects of the mixing/reacting zone structure on the resulting gain region are studied. It is assumed that the flow is laminar and the water vapor condensation due to the supersonic cooling is ignored. A chemical kinetic model encompassing 21 chemical reactions and 10 chemical species is used to determine the chemical composition of the gas mixture. The present results demonstrate that a pair of contrarotating vortices generated behind the I_2 jet greatly enhances the mixing and the simultaneous chemical reaction to produce the excited iodine atom with the singlet oxygen. In the present calculation, the small signal gain coefficient is overestimated to some extent as compared with the experimental one. It is thought that the overestimation is caused by the imperfect chemical kinetic model as well as by ignoring the water vapor condensation and the boundary layers on the upper and lower wall in the present calculation.

Key Words: Supersonic Flow, Reactive Flow, Chemical Laser, Iodine, Oxygen, Numerical Simulation

1. Introduction

The chemical oxygen-iodine laser (COIL) is the only electronic transition chemical laser existing to date. Its wavelength ($\lambda=1.315\ \mu\text{m}$) which is shortest among chemical lasers is suitable for transmission using optical fibers. In addition, its efficiency and the laser power can be increased significantly by the introduction of gas cooling through supersonic expansion^{(1),(2)}. Therefore, a great deal of effort has been made to develop the supersonic flow chemical oxygen-iodine laser (S-COIL). The performance characteristics of the S-COIL have been also studied theoretically in many papers⁽³⁾⁻⁽⁷⁾.

The performance of the S-COIL depends

significantly on its ability to mix molecular iodine gas adequately into the flow of singlet delta oxygen $O_2(^1\Delta)$ from the chemical oxygen generator and to create a favorable gain region from which the optical energy can be extracted. To do this, the molecular iodine I_2 is injected transversely into the subsonic primary flow as shown in Fig. 1. Then, the flow in which I_2 mixes and reacts with $O_2(^1\Delta)$ is choked and expanded through supersonic nozzle blades. As a result of mixing, energy is transferred from the $O_2(^1\Delta)$ to high vibrational levels of the molecular iodine.

where I_2 is the vibrationally excited ($\nu \sim 40$) iodine molecule. Further collisions transfer sufficient energy to dissociate the iodine.

Then, the electrically excited iodine atom $I(^2P_{1/2})$ is produced.

The laser emission can be obtained from a resonator located downstream of the nozzle blades by

where h is the Planck's constant and ν is the frequency. Since the forward reaction rate of the

* Received 4th March, 1996.

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reaction (3) is raised by lowering the temperature, supersonic cooling can enhance the laser emission strongly.

In most high-power S-COILs, the flow field is highly three-dimensional, since the iodine is injected into the primary flow through many circular orifices as shown in Fig. 1. However, the performance characteristics of the S-COIL have been analyzed mostly using some simple mixing models^{(3),(4)} or by solving the two-dimensional Navier-Stokes equations^{(5)–(7)}. Only a few papers^{(8),(9)} have dealt with the S-COIL flow three-dimensionally. Since the chemical reaction and the small signal gain coefficient greatly depend on the mixing process, a precise simulation is indispensable in order to inquire deeply into the performance characteristics of the S-COIL. In the present paper, the flow field of the S-COIL is simulated by solving the three-dimensional full Navier-Stokes equations and the effects of the mixing/reacting zone structure on the resulting gain region are discussed.

2. Mathematical Modeling and Numerical Method

Water vapor is produced in the chemical oxygen generator as an undesirable by-product. In previous papers^{(6),(7)}, the authors demonstrated that the condensation of water vapor due to the supersonic cooling reduces the small signal gain coefficient. For simplicity, however, the condensation is ignored in the present simulation. It is reasonable to assume that the flow is laminar, since the Reynolds number of the S-COIL based on the nozzle throat conditions and the throat height is at most 10^4 , and one based on the orifice diameter of the I_2 injector and the injection condition is only on the order of 10^2 . Moreover, the compressibility and rapid acceleration of the nozzle tend to stabilize the flow.

In addition to the above assumptions, the following simplifications are introduced to derive the governing equations: 1) The laser emission is not considered in the present analysis. 2) The gas mixture consists of ten species: $O_2(^1\Sigma)$, $O_2(^1\Delta)$, $O_2(^3\Sigma)$, $I(^2P_{1/2})$, $I(^2P_{3/2})$, I_2^* , I_2 , H_2O , Cl_2 , He . 3) The specific heat is constant and the equation of state for an ideal gas is used for each species. 4) The bulk viscosity, Soret effect, Dufour effect and diffusion due to the pressure gradient are neglected. 5) External forces such as gravity are neglected. Based on these assumptions, the governing equations, the full Navier-Stokes equations with a detailed chemistry mechanism, are given in the conservative form.

In the present calculation, a chemical kinetic model proposed by Perram and Harger⁽¹⁰⁾ is used to evaluate the chemical composition of the gas mixture. The model consists of the 10 species and 21 chemical

reactions. The recombination of iodine atom and the deactivation of excited species on the wall are not considered in the model.

The molecular viscosity and thermal conductivity coefficients for each species are calculated by the generalized kinetic-theory formula and the Eucken correction⁽¹¹⁾. The mixture viscosity and thermal conductivity coefficients are obtained from the Sutherland-Wassiljewa formula and the Wilke approximation⁽¹²⁾. The effective diffusion coefficients and the binary diffusion coefficients for each chemical species are given by the Chapman-Cowling empirical formula.

The governing equations in the physical domain are transformed to the computational domain and discretized using the cell-centered finite volume method⁽¹³⁾. The higher-order Roe's flux difference splitting scheme with the monotone upstream-centered schemes for conservation laws (MUSCL) approach and van Albada's limiter is 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.

2.1 Numerical conditions

Figure 1 shows the configuration of nozzle blades and iodine injectors adopted for the present calculation. The nozzle blade is the same as one used in a previous experiment^{(2),(5)}. A cylindrical I_2 injector is located upstream of each nozzle blade. In the previous experiment^{(2),(5)}, the secondary I_2 gas was injected into the primary flow through 4 rows of circular orifices drilled in each cylinder. In the present calculation, however, only 2 rows of orifices are used for injection in order to investigate the basic characteristics of the mixing/reacting zone structure clearly. It is assumed that all of the I_2 jets have the same shape and that each jet has a symmetric plane which parts the orifice in the center. The computational domain indicated by the broken lines in Fig. 1 is used in the present calculation. In Fig. 1, the x axis is a coordinate parallel to the primary flow with its origin at the nozzle exit plane, and the y and z axes are coordinates perpendicular to x . The z coordinate is parallel to the cylindrical I_2 injector.

The whole computational domain is separated into three subdomains—the region of the primary flow, near the injector and downstream of the nozzle blade—to enable the grid system to fit the complicated shape. The domain includes 128 800 cells, and the smallest cells are located near the orifice of the I_2 injector and the wall of nozzle blade.

The wall boundary conditions are isothermal,

Streamline
Stream Tube

Fig. 2 Flow field near the I_2 injector: (a) the streamlines and the cross sections of the stream tube issuing from the upper half of the orifice, (b) Mach number contours, (c) $I(^2P_{3/2})$ molar fraction contours, (d) $I(^2P_{1/2})$ molar fraction contours and (e) I_2 molar fraction contours on some planes perpendicular to the jet centerline

contracts owing to the interaction between the expansion wave and a conical shock wave formed from the circumference of the orifice. Successive, but weaker,

expansions and contractions along the jet path can also be observed in Fig. 2(a). The Mach number contours in Fig. 2(b) and Fig. 3(b) show that the

Fig. 3 Flow field downstream of the nozzle inlet: (a) the cross-sections of the stream tube issuing from the upper half of the orifice, (b) Mach number contours, (c) $I^2P_{3/2}$ molar fraction contours, (d) $I^2P_{1/2}$ molar fraction contours, (e) I_2 molar fraction contours and (f) small signal gain coefficient contours on some planes perpendicular to the jet centerline

supersonic flow is maintained along the central portion of the jet. The flow near the side boundary of the jet loses momentum in the injection direction very rapidly due to the strong shear force and deviates from the jet centerline. Therefore, the cross section of the jet is stretched significantly and a pair of contrarotating vortices are formed behind the curved jet. Several branches which are likely to originate from the series of expansions and contractions of the jet near the orifice are observed in the stretched cross section of the jet. Such flow features are conserved far downstream from the I_2 injector as shown in Fig. 3(a). The figure also shows that the multiple jets do not join each other and the primary flow can pass through the multiple curved jets within the computational domain. The calculated ratio of the molar flow rate of the secondary flow to that of the primary one is 0.328. Careful observation of Fig. 2(b) shows that the primary flow passing through the jets very close to the orifice is choked. However, the Mach number decreases and the flow becomes subsonic in a very short distance. The whole primary flow except the boundary layer is choked near the nozzle throat. The boundary layer of the nozzle blade and the wake issuing from the blade are clearly observed in Fig. 2(b) and Fig. 3(b).

The distributions of the molar fractions of the chemical species near the I_2 injector are shown in Figs. 2(c) to (e). It can be seen that substantial iodine molecules are transported far from the jet centerline by the pair of contrarotating vortices. The dissociation to the iodine atom $I(^2P_{3/2})$ occurs at the front boundary of the iodine jet where the singlet oxygen $O_2(^1\Delta)$ primary flow collides with the jet. Then, the partially dissociated iodine jet is engulfed with the singlet oxygen by the vortices and further reaction produces the excited iodine atom $I(^2P_{1/2})$ in the cores of vortices. These results clearly demonstrate that the vortices behind the curved jet greatly enhance the mixing and the simultaneous chemical reaction.

Figures 3(c) to (f) show the distributions of the molar fractions of $I(^2P_{3/2})$, $I(^2P_{1/2})$, I_2 and the small signal gain coefficient downstream of the nozzle inlet. The small signal gain coefficient G is calculated from the resulting flow field:

$$G = \frac{7}{12} \sqrt{\frac{\ln 2}{\pi}} \frac{A}{4\pi} \frac{\lambda^2}{\Delta\nu} \left\{ n[I(^2P_{1/2})] - \frac{g[I(^2P_{1/2})]}{g[I(^2P_{3/2})]} \times n[I(^2P_{3/2})] \right\} \quad (7)$$

where A denotes the Einstein coefficient, $\Delta\nu$ is the Doppler broadening, n is the number density of each species and g means the degeneracy of each species. In these figures, $I(^2P_{3/2})$ is densely distributed in the central portion of the jet. On the other hand, $I(^2P_{1/2})$

Fig. 4 Distribution in the x direction of small signal gain averaged on each plane perpendicular to the x axis. The broken line corresponds to the increased rate constant⁽⁴⁾, while the solid line corresponds to the Perram's reaction model⁽¹⁰⁾ in the figure

is spread out in the computational domain by the vortices. The mixing/reacting zone structure induced by the vortices near the injector is preserved even in the region downstream from the nozzle blade. These results clearly demonstrate the important effect of the vortices behind the iodine jet on the laser performance. The calculated signal gain coefficient is widely distributed and comes up to 3 m^{-1} in the region engulfed by the vortices. It is noted, however, that some amount of I_2 remains in the central portion of the jet because the singlet oxygen $O_2(^1\Delta)$ sufficient to dissociate I_2 completely cannot be provided there. Consequently, the small signal gain coefficient there cannot attain a positive value. Therefore, further improvement of the mixing conditions is indispensable to attaining higher laser performance.

The distribution in the x direction of the small signal gain coefficient averaged on each plane perpendicular to the x axis is shown in Fig. 4. The averaged small signal gain coefficient is about 1.5 m^{-1} downstream of the nozzle blade. In the previous experiment^{(2),(5)}, the measured small signal gain coefficient downstream of the nozzle blades was about 0.9 m^{-1} . Since the configuration of the I_2 injector of the present calculation is definitely different from the experiment, the calculated gain cannot be compared directly with the measured one. However, it seems that the present calculation overestimates the small signal gain coefficient to some extent. There are several plausible sources for the overestimation. The height (in the z direction) of the cross section of the experimental facility was only $12 \text{ mm}^{(2),(5)}$. Therefore, the boundary layers which develop along the upper and lower walls may greatly raise the temperature and reduce the gain. In addition, the condensation of

water vapor ignored in the present calculation has a negative effect on the performance characteristics of the COIL^{(6),(7)}. The imperfect chemical kinetic model and reaction rate constants used in the present calculation may also cause the overestimation of the gain. In fact, the mechanism by which I₂ is dissociated is not understood very well⁽¹⁵⁾. Carroll⁽⁴⁾ increased the rate constant of the deactivation of I₂^{*},

by an order of magnitude in order to get a reasonable agreement between his calculation and experimental data. The increased rate constant in the reaction (8) delays the I₂ dissociation, raises the temperature and increases the consumption of O₂(¹Δ). In the present calculation, increasing the rate constant by a factor of 10 reduces the small signal gain coefficient by 0.3 m⁻¹, as shown in Fig. 4.

4. Conclusions

A numerical simulation of a supersonic flow chemical oxygen-iodine laser has been performed solving three-dimensional Navier-Stokes equations and the effects of the mixing/reacting zone structure on the resulting gain region have been studied. It was shown that the flow near the side boundary of the I₂ jet loses momentum in the injection direction very rapidly due to the strong shear force and deviates from the jet centerline. Therefore, the cross section of the jet from the orifice is stretched significantly and a pair of contrarotating vortices are formed behind the curved jet. The vortices greatly enhance the mixing and the simultaneous chemical reaction transporting substantial iodine molecules far from the jet centerline. Such mixing/reacting zone structure induced near the injector is preserved even in the region downstream from the nozzle blades. These results clearly demonstrate the importance of the pair of contrarotating vortices behind the jet. In the present calculation, the small signal gain coefficient is overestimated considerably as compared with the experimental one. It is thought that the overestimation is caused by the imperfect chemical kinetic model as well as by ignoring the water vapor condensation and the boundary layers on the upper and lower wall in the present calculation.

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