Simulation Mass Flows quantum level spectroscopy in Nozzles for applications in Gas lasers

MOHAMMEDI FERHAT, LAGGOUN CHAOUKI
LARHYSS Laboratory Research Group of Laser Engineering Physics B.P145.R.P 07000,
University of Biskra, ALGERIA

Abstract: The main objectives of work in this area are, first, obtaining the high laser energies in short time durations needed for the feasibility studies of laser induced thermodynamically exothermic CLs chemical, second, investigating the physical principles that can be used to make laser sources capable of delivering high average powers. But the chemical laser makes use of the only chemical reaction in order to generate the excited atoms or molecules at a high temperature. It is the advantage to help the considerable amount of chemical energy from the chemical reaction to form the excited atoms or molecules, which make the chemical laser, have considerably high efficiency of energy transformation and generate high power laser beam. The feasibility and effectiveness of the proposed method is demonstrated by computer.

Keywords: laser, modelling, simulation, gas, nozzles

Received: July 17, 2022. Revised: June 14, 2023. Accepted: July 17, 2023. Published: August 28, 2023.

1. Introduction

Chemical lasers offer the obvious advantage that the population inversion is produced by selective chemical reactions; Chemical compounds are able to store large amounts of energy that may be partially released in exothermal chemical reactions, i.e. the ones proceeding with liberation of energy. It has been rather attractive to convert this energy into coherent optical radiation. Here are some examples of the substitution reactions useful for lasing action (* indicates an excited state). The deuterium fluoride chemical transfer laser, here we give a short exposition to a chemical transfer laser operating in CO2 lines excited by the reaction between deuterium and fluoride. The reactor chamber of the laser, shown in Fig. 1, receives through one port a mixture of helium (carrier gas) and molecular fluorine, and through another port a mixture of nitrogen monoxide and carbon dioxide, The reaction is: The simple chain reaction. Consider the kinetics of
the following chain process:

Initiation of a chemical reaction:
$NO + F_2 \rightarrow NOF + F$, and
an elementary act of reaction, not leading to inversion:

F+H2→ HF*+H

an act of reaction leading to inversion:

$$\begin{array}{c} F+D2 \rightarrow DF^*+D \\ H+C12 \rightarrow HCl^*+Cl \\ Cl+HI \rightarrow HCl^*+I \end{array} \quad (1)$$

a relaxation process
Therefore, the chemical reaction should be not only initiated but also maintained by creating new chemically active species instead of those eliminated from the chain. The number of lasing species also declines through the processes deactivating the upper laser level. Under equilibrium conditions the ratio of the number of molecules in an upper and lower state are given by the Boltzmann distribution:

$$\frac{N_u}{N_L} = \frac{g_u}{g_L} \exp(-\Delta E / KT) \quad (2)$$

This then leads to the concept of partial inversions characterized by vibrational and rotational "temperatures." For a diatomic molecule, in the harmonic oscillator-rigid rotator approximation the energy levels are given by:

$$E(v, J) = \omega_e (v + 1/2) B_r J(J+1) \quad (3)$$

1.1. Governing equations

The following hypotheses are considered for the nozzle problem formulation. A numerical simulation is presented for investigating the effects of two-dimensional equilibrium flow, in viscid flow (where the dissipative transport phenomena of viscosity, mass diffusion, and thermal conductivity are neglected), there is no body force acting on the fluid and there is no heat addition. The development of the following equations is detailed in Anderson [1, 5], and the main steps are described below. At a given location, a gas is characterized by the fluid parameters and the relative mole fractions of the gas components. Variables include (1) static temperature T, (2) static pressure P, (3) density ρ, and (4) gas velocity U. Knowledge of the stoichiometry allows one to also calculate the average molecular weight W, the heat capacities at constant pressure CP and temperature CV, the specific heat ratio γ=CP/CV, and the speed of sound c. When considering the evolution of kinetic processes, one simply uses the velocity U to relate position and time, using dx = Udt. At high velocities, where compressibility of the gas becomes significant, the flow behaviour becomes complicated. This regime is usually defined to occur

when the Mach number, M = U/c, becomes greater than ~0.3. For the case of a no reacting flow with neither friction nor heat addition (isentropic), the flow is characterized by its stagnation properties, which correspond to flow conditions after the flow is isentropically brought to rest, given by:

$$\frac{T_0}{T}=1+\frac{k-1}{2}M^2,\ \frac{p_0}{p}=(1+\frac{k-1}{2}M^2)^{k/(k-1)},\ \frac{\rho_0}{\rho}=(1+\frac{k-1}{2}M^2)^{1/k-1} \quad (4)$$

If the above equations are applied at the throat where M =1, the critical area signified by an asterisk, (*) superscript, the energy equation takes the forms

$$\frac{T^*}{T_0}=\frac{2}{K+1},\ \frac{p^*}{p_0}=(\frac{2}{k+1})^{k/k-1},\ \frac{\rho^*}{\rho_0}=(\frac{2}{k-1})^{1/k-1} \quad (5)$$

where P, T, and ρ are the static properties and P0, T0, and ρ0 are the stagnation properties. Gas flows that travel isentropically through a duct with variable cross section A satisfy Equations

$$(\frac{A}{A^*})^2=\frac{1}{M^2}\left[\frac{2}{k+1}(1+\frac{k-1}{2}M^2)\right]^{k+1/k-1} \quad (6)$$

Equations (7-9) and (10-11) are the characteristic equations and are solved by finite differences. Gas flows that travel isentropically through a duct with variable cross section A satisfy Eq.

$$\frac{dU}{U}=(\frac{dA}{A})/(M^2-1) \quad (7)$$

This expression illustrates the principle of operation behind the converging-diverging nozzle that is widely used in laser applications. In the converging section, the flow accelerates until it reaches the minimum area throat location, where the flow reaches M = 1. It then continues to accelerate beyond the throat in the expanding region, where M continues to increase to supersonic values, resulting in much lower pressure, static temperature, and density. The Mach number, temperature, and pressure dependence of the gas mixture as a function of position in a typical laser cavity with and without the addition of heat due to the secondary flow. The flow rate downstream of the nozzle is as high as 1200 to 1500 m/s (4 to 5 mach number). The excited CO2 molecules lase in the working chamber. Then the gas flow meets the diffuser provided for decelerating the flow and matching its pressure with the atmosphere (see fig.1). The behaviour of the population for states (001) and (020) of the CO2 molecule passing from the prechamber (exothermic reactions) to the working volume ,and simulation fig. 1-4. In the transition region around the nozzle, the (020) level is almost completely removed to the ground state, while state (001) suffers only insignificant loss of its population. As a result, a population inversion occurs between these states.

2. Simulations Conditions

The validation of
the nozzle code developed here was done for the same nozzle geometry described above considering only the air with no chemical reactions, with the ratio of specific heats (k=CP/CV) equal to 1.4. A set of Matlab programs for computing flow properties for the one-dimensional isentropic flow of an ideal gas in figures 1-5:

-Stagnation Properties as Functions of M

-Duct Area Relationship for a Converging-Diverging Nozzle

-Mass a Function of Stagnation Properties

-Mass a Function of Area Ratio

Under the simulation conditions , the transit time of fluid through the laser cavity is about 24 μm sec, compared with 8μm sec resonant transfer time between CO2 and DF (v=1), and 75μm sec relaxation time of the upper laser level. Relaxation time (010) → (000) is in the order 10μm sec.

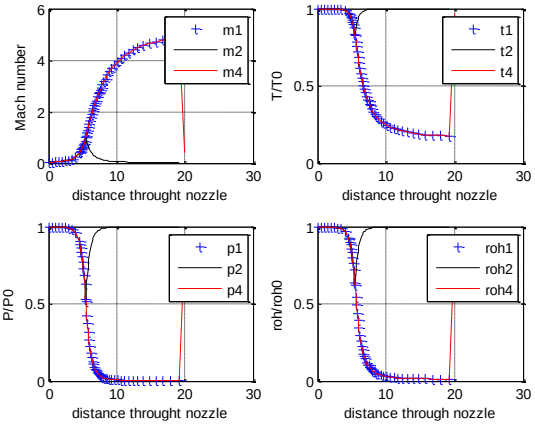

Fig.1-2, Temperature and Mach number distribution inside the nozzle convergent-divergent Nozzle.

The gas equation of state, which is usually well approximated by the ideal gas law, allows calculation of the mass density and local molecular concentrations of the various gas constituents based on temperature and pressure. The classical governing equations can be written in the conservation form as Continuity equation (mass conservation equation)

$$\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=0 \quad (8)$$

Themselves, thus the basic set of equations are unsteady, two-dimensional form of laminar Navier-Stokes equations, augmented with appropriate species continuity, global continuity, energy, state equation and the vibrational relaxation equations, which can be expressed as:
Conservation of species equation.

$$\frac{\partial(\rho X_i)}{\partial t}+\frac{\partial(\rho u X_i)}{\partial x}+\frac{\partial(\rho v X_i)}{\partial y}=\omega_i W_i, i=1,\ldots,N \quad (9)$$

Equation of state

$$p = \rho \Re T \sum_{i=1}^{N} \frac{X_i}{W_i} \quad (10)$$

In the above equations, ρ, p and T are the density, the static pressure and temperature, R̂ is the universal gas constant, ωi and Wi are the net reaction rate and the specific weight of the ith species and N is the total number of species of the system. Considering i as the indices of the species (with a total of N) and k as the indices of the reactions (with the total of K), the expression for the net production rate wi , for the ith species can be written as

$$\omega_i = \sum_{k=1}^{K} v_{ik} q_k \quad (11)$$

Where vik is the stoichiometric coefficient (stoichiometric mole number) of the ith species and the kth reaction. To sum up, the chemical laser spends the energy stored in the vibrational degrees of freedom 'of the molecules arriving at the nozzle as follows. The fraction of the energy stored in the symmetric stretching and bending oscillations of the CO2 molecules converts into the translation energy of the flow leaving the nozzle. The energy stored in the asymmetric stretching oscillations of the CO2 molecules and, what is more important, in oscillations of the HF-DF a molecule converts (minus losses in the resonator) into the energy of the coherent radiation of the lase (see fig.3). The transition (001) → (100) yields a line at the wavelength λ= 10.4 μ m, whereas the (001) → (020) yields a line at λ = 9.4 μ m. The population of the (001) state builds up through inelastic collisions of the CO2 molecules with electron (electron impact) produced in the plasma of the discharge and with the excited nitrogen molecules (resonant energy transfer).

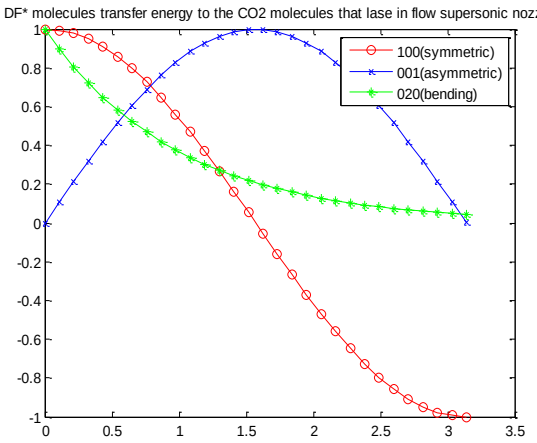

Fig.3- the population of the collisions of the CO2 molecules with the excited nitrogen molecules (resonant energy transfer)

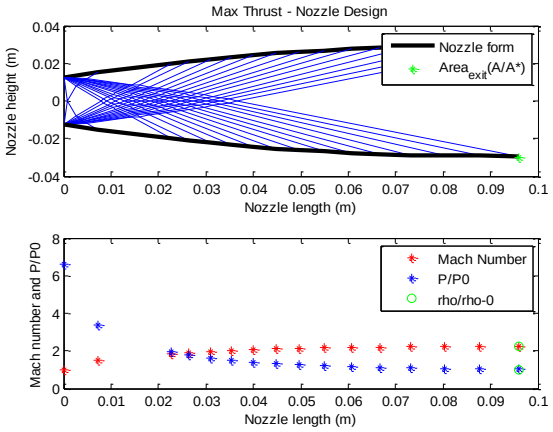

fig 4-5.Flow conditions behind an oblique shock wave for the free stream Mach number

The validation of the nozzle code developed here was done for the same nozzle geometry described above considering only the air with no chemical reactions, with the ratio of specific heats (γ=CP/CV) equal 1 to .4. The region of interest for the present analysis starts from the nozzle exits extends downstream and remains confined between two centerlines severally transitions. This region for the sake of simplicity is referred as duct see figures 1-2 and 4-5. A supersonic stream of vibrationally excited pure chemical reaction HF-DF is mixed tangentially with a supersonic stream of cold CO2, at the nozzle exits. Due to mixing through molecular collisions, vibrational energy is transferred from DF (v=1), to cold CO2 with resonance transition transfer energy see figure 4. Under the simulation conditions , the transit time of fluid through the laser cavity is about 24 μm sec, compared with 8μm sec resonant transfer time between CO2 and DF (v=1), and 75μm sec relaxation time of the upper laser level. Relaxation time (010) → (000) is in the order 10μm sec. Thus, the mass flow only depends on the condition of the gas upstream of the nozzle and its properties. The coefficients of loss of well finished nozzles are today so well known that for the purpose of calculating the mass flow, the motive nozzles of jet pumps supply far more accurate values than any other form of throughput measuring. Therefore motive nozzles can be directly used for the exact.

References

[1]. Anderson J D Jr 1976 Gasdynamic lasers: An introduction (New York: Academic Press)

[2]. Herbst, L., Simon, R., Paetzel, R., Chung, S.-H., and Shida, J.: "Advances in Excimer Laser Annealing for LTPS Manufacturing," IMID, 2009.

[3]. Delmdahl, R., Weissmantel, S., and Reisse, G.: "Excimer Laser Deposition of Super Hard Coatings," SPIE Photonics West, 7581, 2010.

[4]. Usoskin, A., and Freyhardt, H. C.: "YBCO-Coated Conductors Manufactured by High-Rate Pulsed Laser Deposition," MRS Bulletin, 29(8): 583–589, 2004.