

Modelling the Cavity of Continuous Chemical Lasers (CCLs) Using Matlab Applications

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ABSTRACT

The subject that concerns us in this work is the numerical simulation and optimal control of equilibrium of the continuous chemical lasers (CCLs). Laser Chemistry: Spectroscopy, Dynamics and Applications are a carefully structured introduction to the basic theory and concepts of this subject. In this paper we present the design and discuss the performances of a continuous DF chemical laser, based on the exothermic reaction: $F + D_2 \rightarrow DF(v, j) + D$

Keywords: Chemical Laser; Spectroscopy Vibrational; Rotational Processes; Lasers Cavity

1. Introduction

The rapid developments in new laser techniques and applications have extended the field of laser chemistry into many other scientific fields, such as biology, medicine, and environmental science, as well as into modern technological processes. This “natural” invasion is a result of the multidisciplinary character of modern laser chemistry. The success of simple models to simulate the kinetic behaviour of gas lasers has amused a lot of interest in the numerical and theoretical study of such systems. Chemical lasers find their origin in the study [1-3] of the radiation emitted from chemical reactions. In many cases such radiation is of thermal origin. Energy levels and transitions; A laser chemical or otherwise, requires a mechanism to populate an excited state at a sufficiently fast rate such that at some time point there are more molecules in an upper (higher energy) state than in a lower. Under these conditions the number of photons produced by stimulated emission exceed those absorbed, and optical amplification or gain will result (See **Figures 1-2**). Under equilibrium conditions the ratio [4,5] of the number of molecules in an upper and lower state are given by the Boltzmann distribution:

$$\frac{N_u}{N_L} = \frac{g_u}{g_L} \exp(-\Delta E/KT) \quad (1)$$

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:

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

The number of molecules in a vibrational state is given by:

$$N_v = \frac{N}{Q_v} \exp\left(\frac{-\omega(V+1/2)hc}{KT_v}\right) \quad (3)$$

In any given vibrational level the rotational level populations are given by:

$$N = n_2 - (g_2/g_1)n_1 \quad (3a)$$

2. Model Formulation

In general the pumping chemical is using a very difficult and complexity; exigent primary cavity (chamber of reactive) and secondary cavity (the laser chamber for reactions). The mixing of flows is accompanied by the exothermic reaction:



The reacting system can be presented in simplified forms as follows process us initiation, pumping reactions, energy exchange reactions [6,7], (see **Figure 3**) termination and stimulated emission. The usual one dimensional flow equations govern the jet, wherein the energy equation includes a loss term due to lasing. The rate equations for HF(v) have the form of radiative transport equation, where ρ is density, u is flow velocity, and $n(v)$ is mole-mass ratio of HF(v). The quantity $\gamma_{ch}(v)$ is a summation over all chemical reactions, including energy transfer reactions, That affect HF(v):

$$\rho u \frac{dn(v)}{dx} = \chi_{ch}(v) + \chi_{rad}(v) - \chi_{rad}(v-1) \quad (4)$$

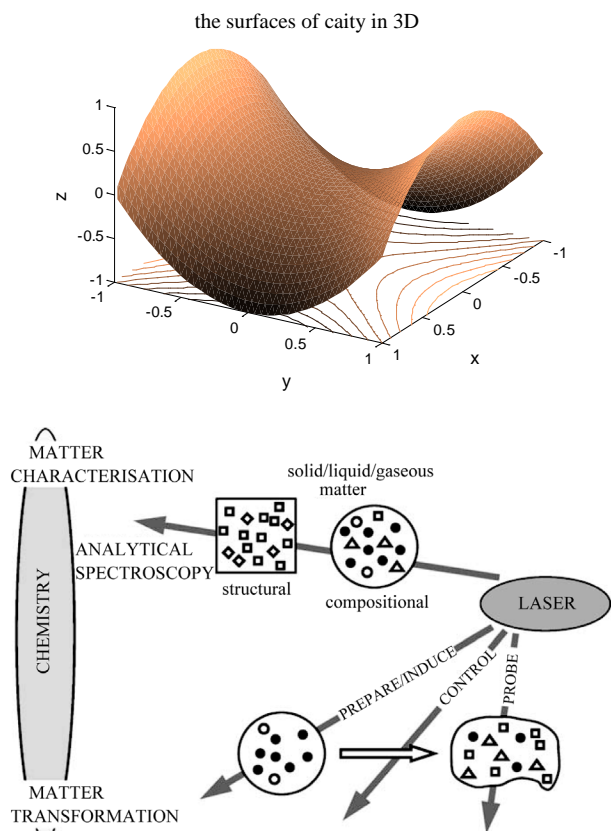


Figure 1. Principle processes in laser chemistry [Telle & All].

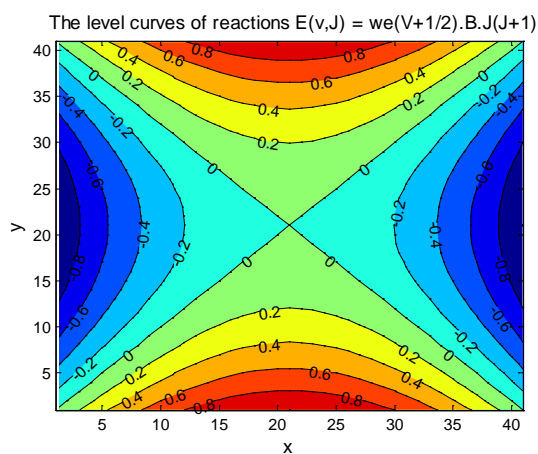


Figure 2. The map surfaces of cavity and curves levels.

$$\chi_{ch}(v) = \sum_r (\beta_{ri} - \alpha_{ri}) L_r \tag{5}$$

$$L_r = K_r \prod_i C_i^{\alpha_{ri}} - K_{-r} \prod_i C_i^{\beta_{ri}} \tag{6}$$

3. Analytical Model

Before you begin to format your paper, first write and save the content as a separate text file. We simulate the

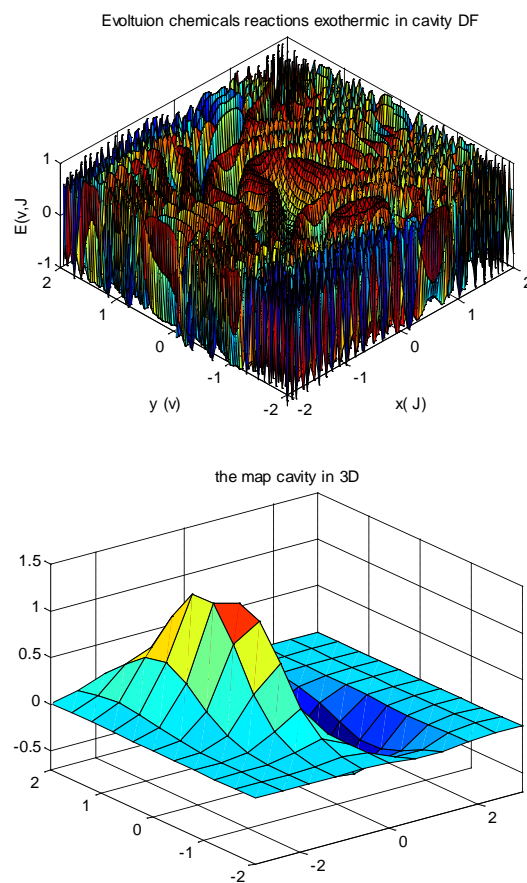


Figure 3. Reactions chemicals in primary and secondary reactions cavity.

differential equations for the density of inversion of laser populations with 3 or on 4 levels, the designations used in this diagram are: ω the probability of transitions stimulated in the channel from oscillation (channel 2-1); ω_p for the radiation of pumping in the channel (1-3); $1/\tau$, the probability of spontaneous transitions in channels 1-3 and 2-3, $n_i(z,t)$ the density of population of the i th level and by n' the total number of active centre per unit of volume. The equations of the assessment for the popula-

tion's n_1, n_2, n_3 have the following equations form Ode's (Ordinary differential equations) [8,9];

$$\begin{aligned}\frac{\partial n_1}{\partial t} &= \omega(n_2 - n_1) - \omega_p(n_1 - n_3) + \frac{n_2}{\tau} + \frac{n_3}{\tau_{31}} \\ \frac{\partial n_2}{\partial t} &= -\omega(n_2 - n_1) + \frac{n_3}{\tau_{32}} - \frac{n_2}{\tau} \\ \frac{\partial n_3}{\partial t} &= \omega_p(n_1 - n_3) - \frac{n_3}{\tau_{32}} - \frac{n_3}{\tau_{31}}\end{aligned}\quad (7)$$

With condition

$$\partial n_1 / \partial t + \partial n_2 / \partial t + \partial n_3 / \partial t = 0 \quad (8)$$

If

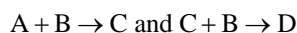
$$n_1 + n_2 + n_3 = n' \quad (9)$$

Then

$$\partial n_2 / \partial t \approx -\partial n_1 / \partial t \quad (10)$$

3.1. ODE's Solvers in MATLAB

A list of ODE solvers and of other routines that act on functions is returned by help funfun, and a documentation window is opened by doc funfun. The two main routines of interest are ODE45, an explicit single-step integrator, and ODE15s, an implicit multistep integrator that works well for stiff systems. We demonstrate the use of ODE45 and ODE15s for a simple batch reactor with the two elementary reactions



The following set of differential equations describes the change in concentration three species in a tank. The reactions $A \rightarrow B \rightarrow C$ occur within the tank. The constants k_1 , and k_2 describe the reaction rate for $A \rightarrow B$ and $B \rightarrow C$ respectively. The following ODE's are obtained:

$$\begin{aligned}\frac{dCa}{dt} &= -K_1Ca \\ \frac{dCb}{dt} &= K_1Ca - K_2Cb \\ \frac{dCc}{dt} &= K_2Cb\end{aligned}\quad (11)$$

where $k_1 = 1 \text{ mn}^{-1}$ and $k_2 = 2 \text{ mn}^{-1}$ and at time $t = 0$, $Ca = 5 \text{ mol}$ and $Cb = Cc = 0 \text{ mol}$. Solve the system of equations and plot the change in concentration of each species over time (Figure 4). Select an appropriate time interval for the integration. We wish to use a general notation system for IVPs, and so define a state vector, x , that completely describe the state of the system at any time sufficiently well to predict its future behavior; The $\text{UF}_6\text{-H}_2$ chemical laser takes advantage of the low moment of inertia of HF and the effectiveness of UF_6 as a photolytic fluorine atom source [15]. Two reactions could

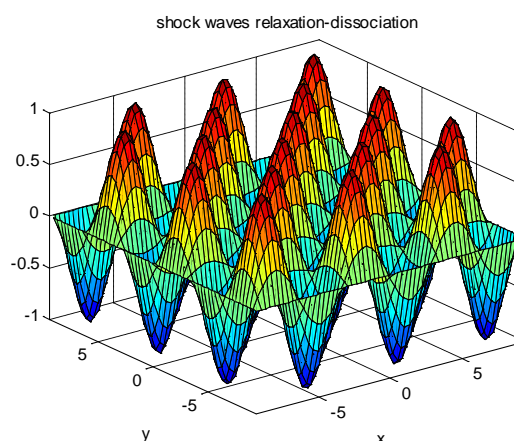
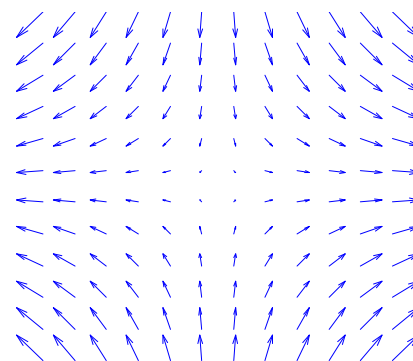
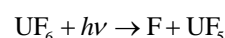


Figure 4. The cavity shock waves relaxation-dissociation.

contribute to the population inversions observed; ($v = 2 \rightarrow 1$ for HF and both $3 \rightarrow 2$ and $2 \rightarrow 1$ for DF).



3.2. Simulation with MATLAB

Systematic Approach: The following reaction data has been obtained from a simple decay reaction; $A \rightarrow B$, Use MATLAB to plot the concentration of component A in mol/L against the reaction time, t , in minutes. Title the plot, label the axes, and obtain elementary statistics for the data. The idea of the simulation part was to form a basic setup for a future test stand for chemical cavities lasers within a numerical routine. The framework for the numerical routine [10,11] has been MATLAB7, a numerical computing environment by "The MATHWORKS", (Figure 5) since it offers a large range of in-built functions and visualization tools. In principle, the very simulations could have been done with any other sophisticated programming environment or language, but the MATLAB language offered the quite comfortable advantage of vector based variables useful for this prob-

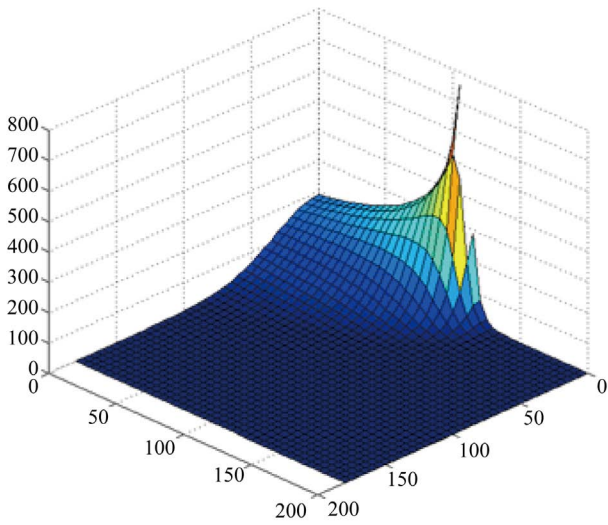


Figure 5. Propagations shock waves in cylindrical lasers cavity.

lem. Cavity parameter variation: Thus, we simulated the work of a continuous chemical $H_2 \rightarrow F_2$ laser with simultaneous lasing on the $V; j-1 \rightarrow v \rightarrow 1, j (j = 14 - 13)$ and $v, j \rightarrow v, j-1 (j = 17 - 16)$ transitions. Suppression of the lasing on vibrational and rotational transitions increased the energy extraction for purely rotational transitions Parameters of simulation cavity: Equations (7), (8) and (11) governing physical phenomena in DF chemical laser cavity is to be discretized. There exist a lot of numerical methods for solving this type of system. Time stepping method, Boundary conditions and the resonator is equipped with two flat mirrors of which separate distances (Fabry-Perrot).

The usual initial conditions for the translation temperature, pressure, density, and Mach number immediately behind the shock are given the Rankine-Hugoniot [12-14] relations (**Figure 6**), State-resolved vibrational kinetics are simulated by the master equation:

$$\begin{aligned} \frac{df_m}{dt} = & \sum_i \left[k_{at}(i \rightarrow m) f_i - k_{at}(m \rightarrow i) f_m \cdot \frac{x_{at}}{\mu_{at}} \cdot \rho \right] \\ & + \sum_{i,j,n} \left[k_{mol}(i, j \rightarrow m, n) f_i f_j - k_{mol}(m, n \rightarrow i, j) f_m f_n \cdot \right] \\ & \times \frac{x_{mol}}{\mu_{mol}} \rho - f_m \frac{1}{x_{mol}} \frac{dx_{mol}}{dt} \\ & - \left[k_{at}(m \rightarrow) f_m - \rho k_{at}(\rightarrow m) \left[\frac{x_{at}}{\mu_{at}} \right]^2 \frac{\mu_{mol}}{x_{mol}} \right] \cdot \frac{x_{at}}{\mu_{at}} \cdot \rho \\ & - \left[k_{mol}(m \rightarrow) f_m - \rho k_{mol}(\rightarrow m) \left[\frac{x_{at}}{\mu_{at}} \right]^2 \frac{\mu_{mol}}{x_{mol}} \right] \cdot \frac{x_{mol}}{\mu_{mol}} \cdot \rho \end{aligned}$$

(13)

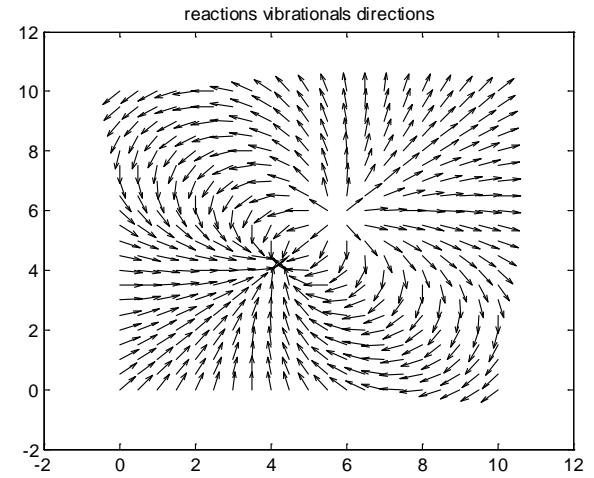
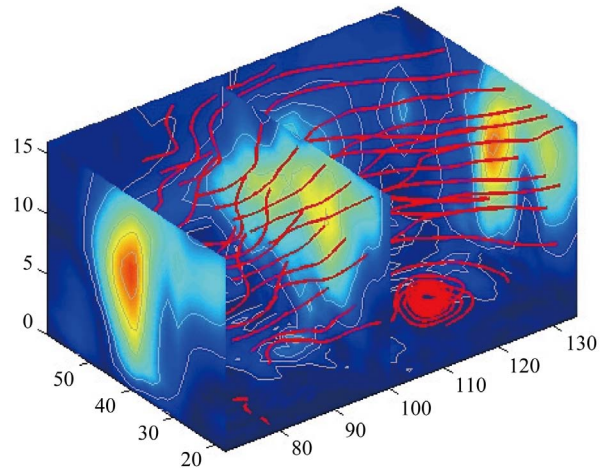


Figure 6. Oscillations shock waves lasers modes in cavity.

The concentration of atoms is given by the equation

$$\begin{aligned} \frac{dx_{at}}{dt} = & 2\mu_{at} \cdot \sum_1 \left[k_{at}(1 \rightarrow) f_1 \frac{x_{mol}}{\mu_{mol}} - \rho \sum_1 k_{at}(\rightarrow 1) \cdot \left(\frac{x_{at}}{\mu_{at}} \right)^2 \right] \\ & \times \frac{x_{at}}{\mu_{at}} \rho + 2\mu_{at} \cdot \sum_1 k_{mol}(1 \rightarrow) f_1 \frac{x_{mol}}{\mu_{mol}} \\ & - \rho \sum_1 k_{mol}(\rightarrow 1) \left(\frac{x_{at}}{\mu_{at}} \right)^2 \cdot \frac{x_{mol}}{\mu_{mol}} \rho \end{aligned}$$

(14)

The last two terms in Equation (13), simulate the vibration-dissociation coupling. $E_{vib}(T)$ and $E_{vib}(t)$ are vibrational energies:

$$E_{vib} = \sum E_v f_v = \sum \omega_e v \cdot [1 - x_e(v+1)] \cdot f_v \quad (14)$$

where f_v can either the equilibrium or a nonequilibrium distribution function.

4. Conclusion

We are now ready to treat more complex problems of greater relevance to chemical engineering practice. We begin with the study of initial value problems (IVPs) of ordinary differential equations (ODEs), in which we compute the trajectory in time of a set of N variables $x_i(t)$ governed by the set of first-order ODEs. We start the simulation, usually at $t_0 = 0$, at the initial condition, $x(t_0) = x[0]$. Such problems arise commonly in the study of chemical kinetics or process dynamics. While we have interpreted above the variable of integration to be time [15-19], it might be another variable such as a spatial coordinate. The following curves is produced upon execution, to be able to solve higher order ODE's in MATLAB, they must be written in terms of a system of first order ordinary differential equations. We have successfully designed, built and tested a in Military applications DF generator for a chemical H-F or DF laser A laser powered by an array of μ SOG chips would be useful for a variety of industrial applications. The comparison of the results of numerical simulations performed with the use of our model with the results of experimental studies.

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