Modelling and numerical simulation of laminar carbon monoxide-oxygen flame impinging on a normal solid surface

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Résumé - *La combustion des carburants fournit fréquemment le chauffage convectif dans l'industrie. Pour prévoir le taux de transfert thermique à partir des flammes aux surfaces solides, les profils de vitesse et le taux de formation massique des différentes espèces sont souvent souhaitables. Dans ce contexte, un modèle mathématique de flamme pré mélangée laminaire dans un écoulement de point de stagnation a été réalisé par la solution numérique des équations de la couche limite. Les équations différentielles partielles qui gouvernent sont transformées en équations différentielles ordinaires par des coordonnées de transformation de similitude, qui sont la forme modifiée de la transformation de Lees. La combustion du carburant qui est le mélange de l'oxyde de carbone et l'oxygène a été modélisée par la réaction chimique élémentaire* $CO + O_2 \Leftrightarrow CO_2+O$*, le système des équations est résolu par la méthode des différences finies.*

Abstract - *Combustion of fuels frequently provides forced convective heating in industry. To predict the rate of heat transfer from such flames to solid surfaces, velocity profiles and mass rate of different species are often desirable. In this context, a mathematical model of laminar premixed flame in a stagnation point flow has been achieved by numerical solution of the boundary layer equations. The governing partial differential equations are transformed into ordinary differential equations by similarity transformation coordinates witch is the modified form of Lees transformation. The combustion of the fuel which is the mixture of carbon monoxide and oxygen was modelled by the elementary chemical reaction* $CO + O_2 \Leftrightarrow CO_2+O$ *the governing system of equations is solved by the finite difference method.*

Keywords: - Combustion - Premixed flame - Stagnation point.

1. INTRODUCTION

Energy conservation and environmental protection have become of prime importance the past few years. One of the most important pollutants in combustion phenomena is carbon monoxide which is a toxic component of air. Catalytic oxidation of carbon monoxide to carbon dioxide at ambient temperature and pressure is an important process for respiratory protection. In particular, the process is widely adopted by mining industries and has also found applications in deep-sea diving, space exploration, and carbon dioxide lasers.

A lot of work is documented on an impinging laminar flame jets. Li *et al.* [1] showed that there exist two different solutions for the flow field in some range of geometric and flow parameters. Heat transfer from an inert jet to a plate has been studied extensively in the past [2], Sibulkin derived a semi-analytical relation for laminar heat transfer of impinging flow to a body of revolution [3], which has been the basis of most other experimental and theoretical results since a important parameter in this relation is the velocity gradient just outside the boundary layer. The present paper

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describes a numerical method for the study of chemically reacting flow in laminar premixed flame of carbon monoxide / oxygen mixture in the region of the stagnation point.

2. DESCRIPTION OF THE PROBLEM

The model being considered is a two-dimensional system in which a laminar premixed flame impinges on a plane solid surface. An exothermic reaction occurs within the jet flow. The general mathematical description consists of a coupled set of differential equations based on the principles of conservation of energy, mass and momentum, and incorporates several chemical rate expressions.

Some of the assumptions adopted in this study are: the thermal conductivity of the solid is taken to be large, the gaseous mixture behaves like an ideal gas whose Prandtl and Schmith numbers are constant and equal to 0.7. The Lewis number is equal to 1, the variation of viscosity with temperature is given by $\mu = c\ T$ where c is a constant, the effects of both thermal and viscous dissipation are neglected. The mass fractions are 80% and 20% for carbon monoxide and oxygen respectively.

A laminar flame impinging on a plane surface is shown in figure 1.

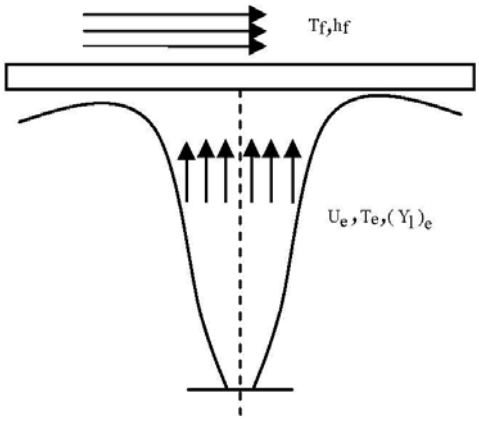

Fig. 1: Flame impinging normal onto a plane surface

2.1 Mathematical formulations

The two most relevant applications of laminar, compressible boundary layer theory are the flat plate flow and stagnation point flow. Both cases give insight into the general effect of compressibility on boundary layer flows and are very useful for estimating the friction and heat transfer on slender bodies or blunt bodies, respectively.

The equations governing the steady, compressible, two-dimensional boundary layer for axisymmetric flow are a coupled set of differential equations based on the principles of conservation of the continuity, momentum, energy, and species. These equations can be written as follow:

Continuity

$$\frac{\partial}{\partial X}(\rho U X) + \frac{\partial}{\partial Y}(\rho V X) = 0 \qquad (1)$$

Momentum

$$\begin{cases} \rho U\dfrac{\partial U}{\partial X}+\rho V\dfrac{\partial V}{\partial Y} = -\dfrac{\partial P}{\partial X}+\dfrac{\partial}{\partial Y}\left(\mu\dfrac{\partial U}{\partial X}\right) \\ \dfrac{\partial P}{\partial X} = \rho_e U_e\dfrac{\partial U_e}{\partial X} \\ \dfrac{\partial P}{\partial Y} = 0 \end{cases} \tag{2}$$

Energy

$$\rho C_p\left(U\frac{\partial T}{\partial X}+V\frac{\partial T}{\partial Y}\right) = \frac{\partial}{\partial Y}\left(k\frac{\partial T}{\partial Y}\right)-\sum_{l=1}^{k} h_l^0\,\omega_l \tag{3}$$

Species

$$\rho\left(U\frac{\partial Y_l}{\partial X}+V\frac{\partial Y_L}{\partial Y}\right) = \frac{\partial}{\partial Y}\left(\rho D\frac{\partial Y_l}{\partial Y}\right)+\omega_I \tag{4}$$

Equation of state

$$P = \rho.R.T \tag{5}$$

Using the following adimensional variable

$$x=\frac{X}{L},\ \overleftarrow{\ }\ y=\frac{Y}{H},\ \bar{\rho}=\frac{\rho}{\rho_e},\ u=\frac{U}{U_e},\ v=\frac{V}{V_e},\ \bar{\mu}=\frac{\mu}{\mu_e},\ h_l=\frac{h_l^0}{C_p T_e},\ \Omega_l=\frac{\omega_l}{a\rho}$$

The boundary layer equations for axisymmetric stagnation point flow will be considered in terms of the boundary layer coordinate [4]:

$$\eta = \beta\int_0^y(\rho/\rho_e)\,dy,\ S=\alpha x^4,\ \Psi=\sqrt{s}\,f(\mu) \tag{6}$$

These transformations coordinates are a modified form of the coordinates first introduced by Lees by combining the Levy and Mangler transformations with Howarth-Doradnitzyn transformations.

By using the definition of stream function Ψ, for a compressible flow, that satisfies the continuity equation (1), by the relations:

$$\bar{\rho}x^2 u = \frac{\partial\Psi}{\partial x},\quad -2\bar{\rho}vyx = -\frac{\partial\Psi}{\partial X} \tag{7}$$

The following are the transformed form of momentum, energy and species boundary layer equations for the stagnation point flow:

Momentum

$$\begin{aligned} &\frac{d^2u}{d\eta^2}+f(\eta)\frac{du}{d\eta}-u^2+\theta = 0 \\ &u = \frac{1}{2}\frac{df}{d\eta} \end{aligned} \tag{8}$$

Energy

$$\frac{1}{Pr}\frac{d^2\theta}{d\eta^2} + f(\eta)\frac{\partial\theta}{\partial\eta} - \sum_{l=1}^{m} h_l \Omega_l = 0 \tag{9}$$

Species

$$\frac{1}{Sc}\frac{d^2 Y_l}{d\eta^2} + f(\eta)\frac{\partial Y_l}{\partial\eta} + \Omega_l = 0 \tag{10}$$

Where: $Pr = \frac{\mu C_p}{k}$ and $Sc = \frac{\mu\rho}{D}$ are Prandtl and Schmith numbers respectively. In these equations, Ω_l is the total dimensionless mass rate of formation of the L^{th} species called the mass source term, and h_l is the dimensionless heat of formation of L^{th} species.

$\sum_{l=1}^{k} h_l \Omega_l$ is called the energy source term.

The term Ω_l is a product of 3 terms:

$$\Omega_L = \sum_{s=1}^{N} D_{L,s} \times F_s(\theta) \times C_s(Y_L) \tag{11}$$

1- A dimensionless group

$$D_{L,s} = W_L \left(v'_{L,s} - v_{L,s}\right) . \left(\frac{P}{R}\right)^{\sum_{L,s}^{m} v_{L,s}^{-1}} . \frac{B_s T_e^{\alpha_s + 1 - \sum_{L,s}^{m} v_{L,s}}}{a . \prod_{L=1}^{m} (W_L)^{v_{L,s}}} \tag{12}$$

Independent of η and which is proportional to the ratio of the characteristic flow time and the chemical time.

2- A function of the dimensionless temperature θ alone

$$F_s(\theta) = \Omega_{L,s} = \theta^{1+\alpha_s - \sum_{L;s}^{m} v_{L,s}} . \exp\left(-\frac{E_s}{\theta}\right) \tag{13}$$

3- A function of the mass fraction Y_L alone

$$C_s(Y_L) = \prod_{L=1}^{m} (Y_L)^{v_{L,s}} \tag{14}$$

So, the problem under consideration is described by the system of equations (8), (9) and (10).

The kinetic model considered is the oxidation of carbon monoxide according to the following stoichiometry: $CO + O_2 \Leftrightarrow CO_2 + O$. The equations are discretized through a finite difference method, for the solution it's necessary to give boundary conditions at the boundary layer edge of the stagnation point flow.

2.2 The boundary layer conditions:

The boundary conditions for the governing equations system are:

$$\eta = 0: \quad f(0) = 0,\ u(0) = 0,\ \frac{d\theta}{d\eta}(0) = Bi(\theta_w - \delta),\ \frac{dY_l}{d\eta}(0) = 0$$

$$\eta = \infty: \quad f(\infty) = 1,\ u(\infty) = 1,\ Y_l(\infty) = (Y_l)_e$$

2.3 Thermodynamic transport proprieties, reaction rates

The reaction model consists of 4 species witch are CO, O_2, CO_2, O, and 2 homogeneous reactions. Their rate parameters are listed in **Table 1**, the model is based on a careful review of recent kinetics literature, and the model is able to predict the flame temperature, fluid velocity, and species concentration profiles.

Table 1: Reaction rate constants [5]

$$K_s = B_s T^{\alpha_s} . \exp(-E_s / R . T)$$

	Reaction	B_{fs} (cm^3/mol.s)	α_{fs}	E_{fs}/R (K)	B_{bs} (cm^3/mol.s)	α_{bs}	E_{bs}/R (K)
1	$CO + O_2 = O_2 + O$	$2.53\ 10^{12}$	0	24000	$2.11\ 10^{13}$	0	26890

2.4 Numerical solution of the problem

A special code is developed to solve numerically the governing equations. It is based on an implicit finite difference scheme the inertia term is linearized through a Taylor series expansion around the previous iteration. A uniform grid is considered. The coordinates η of the nodal point I is given by:

$$\eta = (i - 1) . \Delta\eta \qquad I \le i \le I + 1$$

I is the maximal number of nodal points in the η direction. In order to respect the second order precision, a four nodal point discretisation for the second order derivative and a three nodal point for the first order are performed. We finally use the Gaussian elimination with partial pivoting method to solve the linear algebraic equations systems.

3. RESULTATS AND DISCUSSION

3.1 Velocity and temperature profiles

In this section, we present results of the numerical modeling, figure 2 shows typical profiles for the temperature and velocity in the region of stagnation point, at the boundary mixture temperature T_e = 1300 K, a pressure of 1 atm, a characteristic flow time of 1/300 s. The maximum of temperature exists in front of the surface denoting the location of the flame. It decreases up stream because of the small reaction rate of the carbon monoxide with oxygen, in flow region where the velocity is not affected.

It's well known that the velocity increases with the augmentation of heat if the gaseous mixture, but in this context we can see that the velocity is not affected by the increase of temperature in the jet flow, this can be explained by, first: the values of a characteristic flow time in this case 1/300 s, is faster then the characteristic chemical reaction time, second; the high activation energy for this kind of reaction (values are shown in **Table 1**).

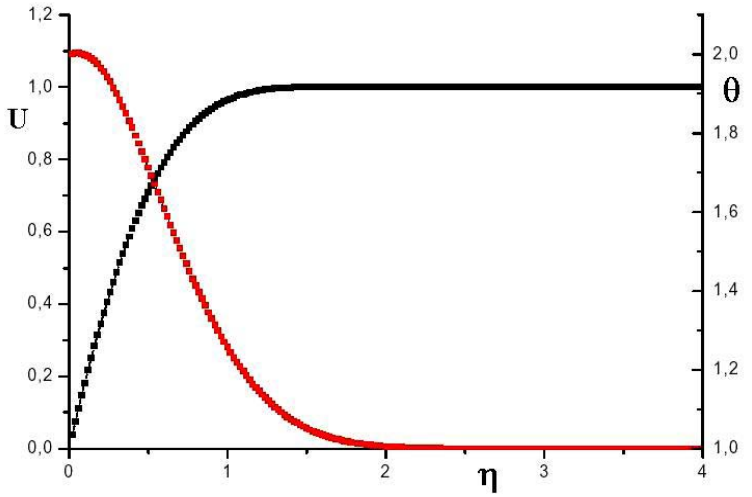

Fig. 2: Velocity and temperature profiles of the flame jet impinging onto plane surface

Because of both factors the inhibition of the flame is highly dependent on the mixture temperature. We can see that the Arrhenius rate expression is proportional to $\exp(E_s / R.T_e)$, the effective activation temperature is monitored along with the characteristic time flow, lower limit is found to be 1300 K.

3.2 Mass fraction profiles

The following figures show the variation of CO, O_2, CO_2 and O in the stagnation point flow. It is clearly seen that the increase of carburant and oxidant witch are carbon monoxide and oxygen leads to the decrease of products CO_2 and O.

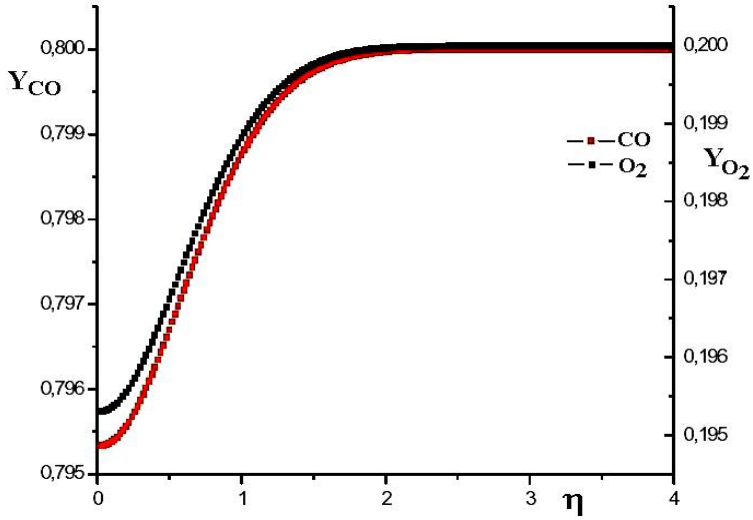

Fig. 3: Mass fraction profiles of CO, O_2 in the stagnation point flow

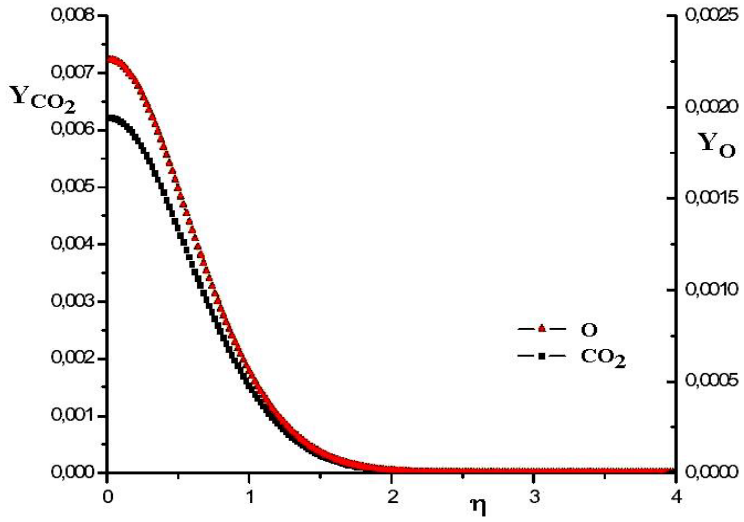

Fig. 4: Mass fraction profiles of CO_2, O in the stagnation point flow

The combustion of carbon monoxide consumes the O_2 to give CO_2 and O, the profiles of all species have a maximum in front of the plane solid surface, where the reaction rate is most important. Our mixture is poor of oxygen, and the reaction rate for the CO and O_2 is known to be slow. It is possible that the slow kinetics of the system requires more time for enough collisions to occur to get complete combustion. The lean reaction rate of this mixture can be explained through three important physical parameters. First, the mass fraction of carbon monoxide and oxygen in the inlet flow; Second; the boundary mixture temperature; Third; the characteristic flow time. The choice of adequate values of these parameters is very important for the ignition of the mixture.

Introduction of hydrogenated corposants such as H_2, H_2O to this mixture [6], confirms that we can get more important reaction rate for lower boundary temperature mixture.

4. CONCLUSION

A numerical study has been performed on a steady stagnation point combustion flow onto a plane solid surface, premixed laminar carbon monoxide-oxygen axisymmetric jet flow was investigated with a simple chemical model which assumes four species in chemical equilibrium; the fluid flow problem has been solved by finite difference method.

A main focus of the present work was to predict velocity, temperature, and different species profiles.

And well understand the effect of different physical parameters on the ignition of the flame.

The choice of adequate values of mass fraction of carbon monoxide and oxygen, the inlet temperature mixture, and characteristic flow time is very important for the ignition of the mixture.

To improve the reaction rate of carbon monoxide/oxygen mixture, the introduction of hydrogenated corposants is very important, that can lead to the ignition of the mixture at low boundary temperature.

NOMENCLATURE

T : Temperature
h : Convective heat transfer coefficient
U :Stagnation velocity flow (X direct.)
Y_l : Mass fraction of species l
S : A new coordinate of similarity
h_l : Enthalpy formation of species l

Greek symbols

η : Non-dimensional normal coordinate
θ : Non-dimensional temperature (T/Te)
α_s : Exponent in Arrhenius low
α , β : Factors similarityTransformations

Subscripts

e : Edge of boundary layer, w : wall

u : Non dimensional velocity
Pr : Prandtl number
Bi : Biot number
Sc : Schmidt number
B_s : Pre exponential factor
E_s : Activation energy
R : Universal gas constant
Ψ : Stream function
ρ : Density
Ω_l : Mass source term

f : fluid, l : species, s : reaction

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