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MODELING AND NUMERIC SIMULATION OF A NON PREMIXED LAMINAR COMBUSTION

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Abstract. *This work presents a comparison between two models of non premixed laminar combustion with different complexity levels. Methane and air are used as fuel and oxidant, respectively. The first method assuming infinitely fast chemistry, adopted for the flame sheet model. The most complex, named Finite rate chemistry model, uses the quasi-global mechanism to describe the chemical reactions. To modeling, a set of differential equations for mass, energy and momentum (two dimensional axisymmetric geometry), unsteady, are solved numerically by a Control Volume Finite Element Method. The numeric code was programmed in MATLAB language. Some results obtained by numerical simulation are compared with experimental data and good agreement is observed for the prediction of temperature, velocity and mole fraction profiles.*

Keywords: *Non premixed combustion, laminar flame, numeric simulation*

1. INTRODUCTION

The combustion process is one of the oldest technologies in the world Warnatz *et al.* (2006). According to Dreizler and Janicka (2007) more than 80% primary energy is converted from combustion and the prevision is to continue at the year of 2020 producing by fossil fuels the same amount. Westbrook and Dryer (1981) points out the flame propagation as a recurrent problem and the chemical kinetic can develop ways to solve it. In some applications it is needed a trustable model which the simplicity are enough to reproduce the experimental phenomenon instead of using complexes models which are good, for example, for pollution analysis.

Great conditions for the non premixed combustion are on the boundary surface of the stoichiometric mixture. It is where fuel and oxidant will be completely consumed. This will lead to the peak temperature and therefore the temperature sensibility of chemical reactions for this reaction rate is faster. In most cases, the combustion is faster than diffusion, so the diffusion will work as the limiting barrier to control the process (Peters, 1992).

Several fuels are mixture and contains many hydrocarbons. Turns (2013) also points out the procedure to modelling combustion is considering one specie or a few species mixture instead of a complex fuel which reproduces the important characteristics, as an example natural gas can be represented by methane.

The obvious advantage, quoted by Flogan and Seinfeld (1988), of the simple mechanism is its simplicity. It is useful for the heat release and flame stability, but do not include intermediate hydrocarbons neither carbon monoxide. Chemical kinect describes well what happens when the fuel burns, but alone cannot describe combustion in a practical form.

The global mechanism reduces the kinect calculation complexity using most of the stable species, in this case CO and H_2. In this paper, we review the Westbrook and Dryer (1981) three steps mechanism considering finite rate and comparing the accordance between Tarhan and Selçuk (2003) flame sheet model considering irreversibility and infinitely fast chemistry with one step, the energy and the mass fraction of chemical species are calculated through mixture fraction. For the calculation was considered equations of mass conservation, momentum conservation, and mass fraction conservation. Lastly, in order to verify the results of a cylindrical chamber combustion simulation, it is checked with experimental data produced by Mitchell *et al.* (1980). In order to fulfill the gaps of time consuming simulation models an simple solutions that do not meet the needs o predicting experimental results, the present work aimed to develop a trustable model which the simplicity is enough to reproduce the experimental phenomenon.

2. MODELING OF LAMINAR NON-PREMIXED FLAMES

2.1 Laminar Fluid Flow

The laminar flow field calculation can be obtained solving the mass conservation equation and momentum conservation equation. For an incompressible and Newtonian fluid flow:

$$\frac{\partial}{\partial t}(\rho)+\nabla\cdot(\rho u)=0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u)+\nabla\cdot(\rho uu)=-\nabla p+\rho g+\nabla\cdot(\mu\nabla u) \tag{2}$$

Where u is the velocity vector and p is the pressure. The density and viscosity of the mixture are represented respectively by ρ and μ. The term ρg is the buoyancy (force experienced in a fluid due to a variation of density in the presence of a gravitational field).

2.2 Finite Rate Chemistry Model

The Finite Rate Chemistry Model considers a finite chemical reaction rate. In general can be assumed that the products are usually not formed by a single chemical reaction step. The rate, which the chemical connection is broken or created, can be represented by a reaction mechanism. In a global reaction mechanism, coming close to combustion, usually is assumed that reactants are converted into final products through few irreversible steps.

For this work, each chemical specie correspond to a conservation equation:

$$\frac{\partial}{\partial t}(\rho Y_k)+\nabla\cdot(\rho u Y_k)=-\nabla\cdot(\mathbf{J}_k)+\dot{\omega}_k \tag{3}$$

The mass fraction is represented by Y_k. The index k denotes a specific chemical species: H_2, H_2O, O_2, CO, CO_2, CH_4, and N_2. The term $\dot{\omega}_k$ characterizes the net rate of production of specie k due to homogeneous reactions. These reaction rates must be obtained from the reaction mechanism. Fick's law will be used in the approximation of the diffusion flux of species, $\mathbf{J}_k=-\rho D_k\nabla Y_k$. The D_k is a term for the diffusion coefficient. In order to simplify, it is assumed unitary Lewis number, $Le=\alpha/D=1$, and because of it, every equal D_k can be determined from: $D=\alpha$.

The mechanism for homogeneous reactions is presented in Tab. 1. The rates constants from Tab. 1 were obtained from Westbrook and Dryer (1984).

Table 1 Global mechanism for homogeneous reaction.

$CH_4+\frac{1}{2}O_2\xrightarrow{R_{CH4}}CO+2H_2$	$R_{CH4}=-A_{CH4}\exp\left(-E_{CH4}/\left(R_uT_g\right)\right)[CH_4]^a[O_2]^b$
$CO+\frac{1}{2}O_2\xrightarrow{R_{CO}}CO_2$	$R_{CO}=-A_{CO}\exp\left(-E_{CO}/\left(R_uT_g\right)\right)[CO]^a[O_2]^b[H_2O]^c$
$CO_2\xrightarrow{R_{CO_2}}CO+\frac{1}{2}O_2$	$R_{CO2}=-A_{CO2}\exp\left(-E_{CO2}/\left(R_uT_g\right)\right)[CO_2]^a$
$H_2+\frac{1}{2}O_2\xrightarrow{R_{H_2}}H_2O$	$R_{H2}=-A_{H2}\exp\left(-E_{H2}/\left(R_uT_g\right)\right)[H_2][O_2]$

For this modelling type, the temperature field is obtained from the energy conservation equation, given by:

$$\frac{\partial}{\partial t}(\rho c_{p,mix}T)+\nabla\cdot(\rho c_{p,mix}uT)=\nabla\cdot(k_{mix}\nabla T)+\Sigma_{k=1}^{Nesp}\dot{\omega}_k h_k \tag{4}$$

Where T is the temperature, the terms $c_{p,mix}$ and k_{mix} represent specific heat and thermal conductivity of the gas mixture respectively. The term $\Sigma_{k=1}^{Nesp}\dot{\omega}_k h_k$ represent the heat generation due to homogeneous reactions.

2.3 Infinitely Fast Chemistry Model (Flame Sheet Model)

When the concern is with the global process combustion and with the final species concentration, one irreversible global specie with infinitely fast chemistry might be used to represents the combustion (Zeng and Chow, 2011):

$$\mathrm{CH_4}+2\eta(\mathrm{O_2}+3.76\mathrm{N_2})\rightarrow\max(0,1\text{-}\eta)\,\mathrm{CH_4}+\min(1,\eta)\,\mathrm{CO_2}+2\min(1,\eta)\,\mathrm{H_2O}+2\max(0,\eta\text{-}1)\,\mathrm{O_2}+7.52\eta\mathrm{N_2} \tag{5}$$

In an explicit form, mass fraction of species can be determined as follows:

$$\mathrm{Y_{CH_4}}(\eta)=\max(0,1\text{-}\eta)\left(W_{\mathrm{CH_4}}/W_{total}\right) \tag{6}$$

$$Y_{CO_2}(\eta) = \min(0,\eta)\left(W_{CO_2}/W_{total}\right) \quad (7)$$

$$Y_{H_2O}(\eta) = 2\min(1,\eta)\left(W_{H_2O}/W_{total}\right) \quad (8)$$

$$Y_{O_2}(\eta) = 2\max(1,\eta-1)\left(W_{O_2}/W_{total}\right) \quad (9)$$

$$Y_{N_2}(\eta) = 7{,}52\eta\left(W_{N_2}/W_{total}\right) \quad (10)$$

$$\eta(f) = \left[(1-f)/f\right](F/A)_{stoich} \quad (11)$$

Which η assume values from 0 to 1 depending on fuel and oxidant concentration. $(F/A)_{stoich}$ is the stoichiometric fuel-air ratio. The total molecular weight can be calculated as: $W_{total}=W_{CH4}+2\eta(W_{CO2}+3{,}76W_{N2})$.

To determine temperature as a function of mixture fraction (f) is needed a calorific state equation. Moreover, to promote similarity between enthalpy and mixture fraction equations, must be written an dimensionless enthalpy. According to Turns (2013), for three flame areas, temperature can be determined:

Inside the flame ($f_{stoich}<f\leq 1$): $$T(f) = f\left[\left(T_{comb,in}-T_{oxid,\infty}\right)-\frac{f_{stoich}}{1-f_{stoich}}\frac{\Delta h_{comb}}{c_{p,mix}}\right]+T_{oxid,\infty}+\frac{f_{stoich}}{1-f_{stoich}}\frac{\Delta h_{comb}}{c_{p,mix}} \quad (12)$$

On the flame $f_{stoich}=f$: $$T(f) = f_{stoich}\left(\frac{\Delta h_{comb}}{c_{p,mix}}+T_{comb,in}-T_{oxid,\infty}\right)+T_{oxid,\infty} \quad (13)$$

Outside the flame $0<f\leq f_{stoich}$: $$T(f) = f\left(\frac{\Delta h_{comb}}{c_{p,mix}}+T_{comb,in}-T_{oxid,\infty}\right)+T_{oxid,\infty} \quad (14)$$

Which $T_{comb,in}$ and $T_{oxi,\infty}$ are fuel and oxidant inlets temperatures, respectively. Furthermore f_{stoich} is the stoichiometric mixture fraction and Δh_{comb} is the methane combustion enthalpy.

As presented, it is not required to solve the individual chemical species equation and also energy conservation equation, all the calculation of the chemical composition and energy conservation is solved as function of mixture fraction. According to Turns (2013), mixture fraction is a passive scalar, that conservation can be determined following the equation:

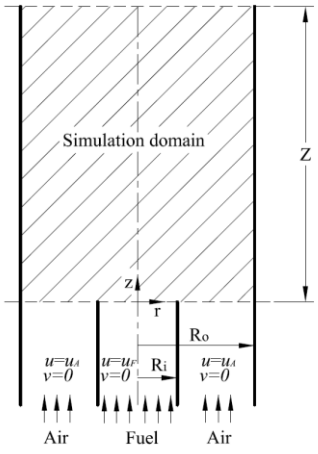
$$\frac{\partial}{\partial t}(\rho f)+\nabla\cdot(\rho u f)=\nabla\cdot(\rho D\nabla f) \quad (15)$$

Mixture fraction is unitary around the fuel inlet and null in the oxidant inlet and chamber walls.

3. SIMULATION, RESULTS AND DISCUSSION

3.1 Test Case

The present laminar flame experimental study, by Mitchell et al. (1975), was the reference for this work. The laminar flame is confined in a vertical axisymmetric cylindrical chamber, with two concentric tubes, radius Ri e Ro, which pass through fuel and air respectively, as shown in Fig. 1.



Fuel inlet
Axial velocity inlet: $u_F=4.5cm/s$
Radial velocity inlet: $v_F=0cm/s$
Temperature: T_F=298K
Mass fraction: $Y_{CH4}=1$
Mixture fraction: $f=1$.
Air inlet:
Axial velocity inlet:: $u_A=9.88cm/s$
Radial velocity inlet: $v_A=0cm/s$
Temperature: T_A=298K
Mass fraction: $Y_{O2}=0.233$ e $Y_{N2}=0.767$
Mixture fraction: $f=0$
Operating Conditions:
Pressure at the exit of the burner: p=101325Pa
Reference temperature: $T_{ref}=T_{wall}=298K$

Figure 1. Vertical cylindrical burner scheme.

According to Mitchell *et al.* (1980) flow rate of fuel and oxidant was adjusted in order to produce a diffusive and steady flame. A cylindrical glass (Pyrex) is used to protect the flame and also to define the system boundary. The intern radius measurement of the fuel jet, Ri, is 0.635 cm and the external radius, the oxidant jet, is 2.54 cm. The chamber is 30 cm high.

3.2 Pre-Processing

Geometry and mesh was designed using Gambit 2.4.6 software. Boundary conditions and initial conditions used to the simulation are in the Tab. 2. The velocity values, temperature, chemical species fraction and mixture fraction at the inlets are in Fig. 1.

The mesh refinement level has a direct effect over the results. In general, refined mesh has better and more accurate results, although the processing time is also bigger. That is why three meshes, with different crescent volume control numbers were used: coarse mesh (6161 control volumes), intermediate mesh (12236 control volumes) e fine mesh (24257 control volumes). Figure 2. shows one of the used meshes. As checked, the reactants region was refined.

Table 2. – Boundary conditions, BC and initial conditions, IC.

			Both methods		Flame Sheet Model (mixture fraction)	Finite Rate Model	
IC	$t = 0$	$\forall z \Lambda \forall r$	$u = 0$	$v = 0$	$f = 0$	Y_{O2}=0,233 e Y_{N2}=0,767	$T=T_{ref}$
BC1	Axis	$\forall z \Lambda \forall r$	$\partial u/\partial r = 0$	$v = 0$	$\partial f/\partial r = 0$	$\partial Y_k/\partial r = 0$	$\partial T/\partial r = 0$
BC 2	Wall	$\forall z \Lambda \forall r$	$u = 0$	$v = 0$	$f = 0$	$Y_k = Y_{wall}$	$T= T_{ref}$
BC 3	Inlet	$\forall z \Lambda \forall r$	$u = u_e$	$v = 0$	$f = f_{in}$	$Y_k = Y_{in}$	$T= T_{ref}$
BC 4	Outlet	$\forall z \Lambda \forall r$	$\partial u/\partial Z = 0$	$\partial v/\partial Z = 0$	$\partial f/\partial Z = 0$	$\partial Y_k/\partial Z = 0$	$\partial T/\partial Z = 0$

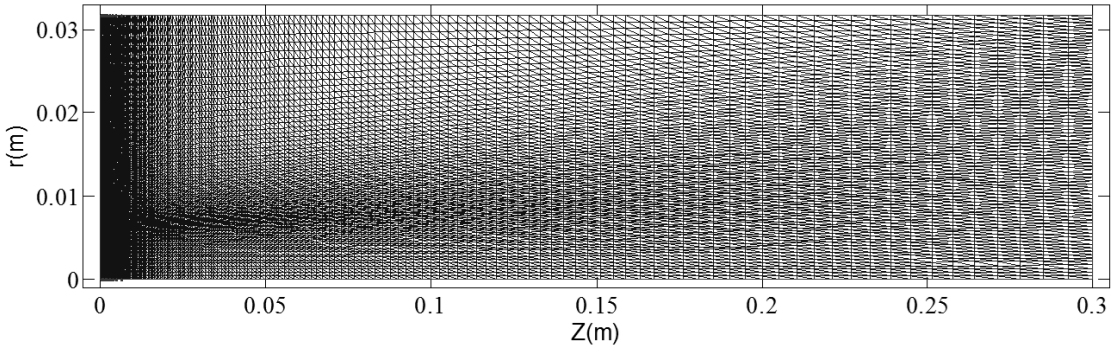


Figure 2. Finite element mesh (12236 control volumes).

3.3 Processing (Solver)

A numeric code has been specially written for the solution of conservation equations for mass, energy and momentum (two-dimensional axisymmetric geometry and unsteady). These equations were discretized using a Control Volume Finite Element Method - CVFEM. CVFEM extends and match the concepts of the finite elements method and the finite volume method (Saabas and Baliga, 1994). It uses control volume unstructured mesh, build normally for the median method from the finite triangle elements mesh. Mass conservation and momentum equations were solved in segregated form, such described at SIMPLE algorithm by Patankar (1980). The numeric code was programmed in MATLAB language. The computer configuration was processor Intel®Core™ i7-3630QM 2.4GHz, 8 GB DDR3 RAM memory and operational system Windows 8.

3.4 Results and Discussion

From now on, the results obtained from the numeric simulation are presented and compared with experimental data of Mitchell *et al.* (1980). Thereby it is verified if the modelling is accurate or not.

Considering flame sheet model, CPU time spent on simulating was 5.89, 10.69 and 23.35 hours, coarse mesh, intermediate mesh and fine mesh, respectively. The obtained results with intermediate and fine meshes were very close, instead, the coarse mesh showed divergent values. Therefore, the chosen one was the intermediate, since it had good results and good processing time, less than half of fine mesh, which proofs being more advantageous for this work.

The CPU time considering Finite Rate Model and intermediate mesh was 144.36 hours. Therefore it is nearly 13.5 times more than the other process. Surely, this attribute must be considered in which modelling will be applied to simulate.

For reasons of space, only one reactant (O_2) and one product (H_2O) of combustion profiles are shown. Furthermore, the chemical reaction is available in terms of moles fraction, therefore the moles fraction (X_k) for each chemical specie, used in profiles comparison, was based on the mass fraction (Y_k) simulated for each specie respectively.

Initiating with results analysis, for the O_2 profiles in Fig. 3, the flame sheet model shows a divergence at the beginning, since the experimental data is not null and irregular, manly for the z=1.2 cm position. Instead, the quasi global result is better and follow much closer the real data and in the most of profiles show good conformity. Not only for the O_2 molecule, but also for the N_2, H_2O and CO_2, as long it moves away from the burner injection entrance, the curve does not show good accuracy, supposedly, as well, because of the mesh thickness. According with Tarhan and Selçuk (2003) and Sauer (2012), this unconformity of O_2 on the fuel side occurs the impossibility for the oxidant to penetrate the other side, since the model does not consider a mixture region. As Westbrook and Dryer (1981) says, the methane oxidation is the most atypical experimental regime from all the n paraffinic fuels.

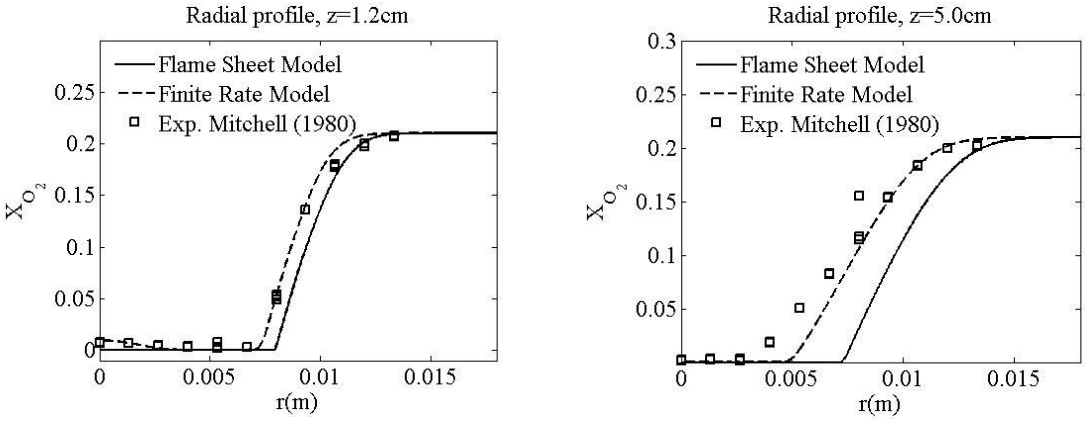


Figure 3. Radial O_2 profiles at z=1.2 cm and z=5.0 cm

H_2O profiles, shown in Fig. 4., rise with the radial length and then lean close to zero with the peak value of 0.2 for the molar fraction, as observed for Du (2000). Mitchell *et al.* (1980) indicates that the experimental data are quite big in behalf of humidity recirculation in the combustion chamber, and despite this fact, both methods could prevent the molecule behavior, with disparity at the beginning values for the quasi global model and in the decay curve, as well as the peak value, for the flame sheet model.

As predicted by Jones and Lindstedt (1988) the carbon monoxide peak values are very unpredictable, which was found the concentration around 1-2% and the typical measure is 4-6% in other papers. In the quasi global some disagreement is resultant of concurrence between the fuel degradation and the branching chain reaction, occurring in an early CO oxidation. In addition to it, this finite rate model have many species and its time reaction is very small. According to Galletti *et al.* (2013) the quasi global method used from WD compared with other detailed kinetics could not prevent the CO levels and suggests some revisions.

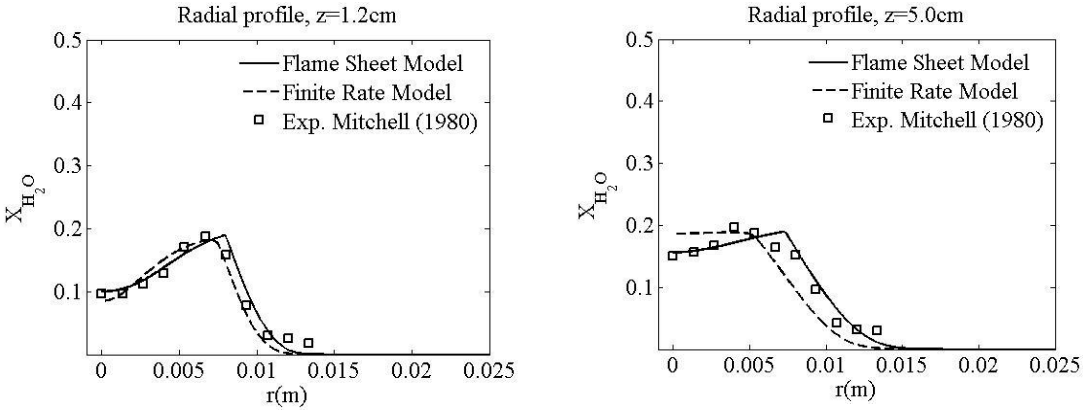


Figure 4. Radial H_2O profiles at z=1.2 cm and z=5.0 cm

Methane analysis are in accordance with Du (2000) and it shows big values difference between experimental and simulation data. Sauer (2012) also says it happens in reason of assumption of Lewis number for all chemical species equals to one. The N_2 profiles match quite well. In general is observed the moles fraction are high at the beginning and follow well the data from the middle to the end.

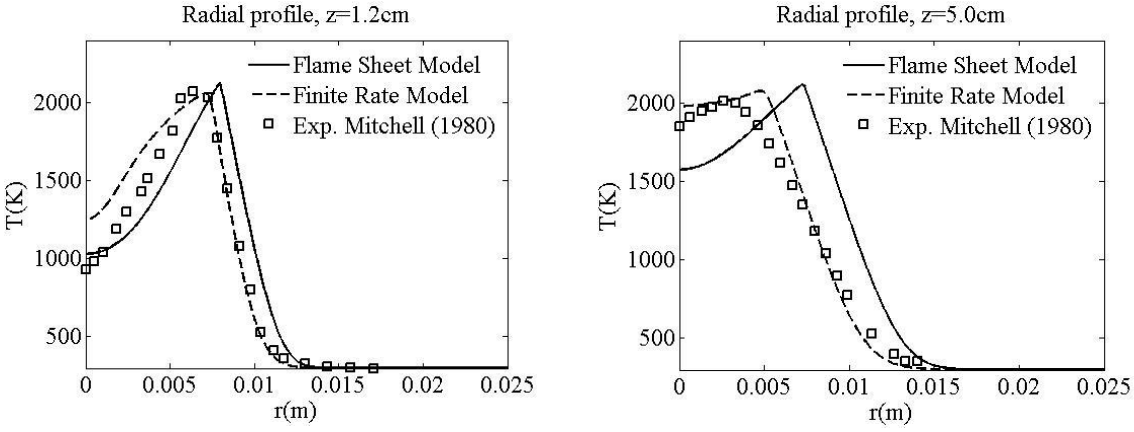


Figure 5. Radial temperature profiles at z=1.2 cm and z=5.0 cm

The radial temperature profiles, shown in Fig. 5, are divergent from the experimental data. Tarhan and Selçuk (2003) consider that this disagreement is caused by approaches of the infinity reactions, used in the flame sheet model.

Flame sheet model take into account infinitely fast reaction and reactants are converted directly into water and carbon dioxide, so that is why it has a higher temperature than the experimental data. Considering finite rate and with CO e H_2 participation in the quasi global model beyond H_2O and CO_2 the flame temperature has a lower peak value, Fig. 5, as predicted by Du (2000). Concerning the time spend on simulation Flogan and Seinfeld (1988) says that the reaction rate applying detailed combustion or the quasi global model always will be extreme slow unless its temperature exceed the critical temperature setpoint.

At low temperatures (<1300 K) the CO consumption is negligible, and this specie is expected to have a weak effect on the reaction under this condition. In high temperatures, the hydrogen atom starts to convert CO_2 to CO, resulting in changes on the CO/CO_2 rate and O/H radical composition, when compared with normal combustion. Andersen *et al.* (2008) says that the WD mechanism cannot predict with accuracy the CO exit, and it changes with temperature.

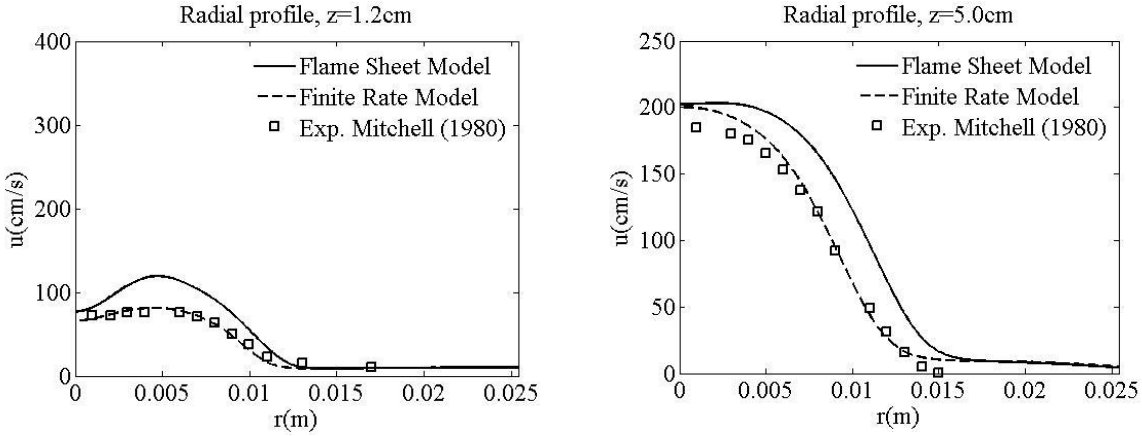


Figure 6. Radial velocity component profiles at z=1.2 cm and z=5.0

Radial velocity profiles and axial ones, Fig. 6 and Fig. 7, respectively, show outlying results for the flame sheet model, as also observed by Tarhan and Selçuk (2003). This also agrees with a higher flame temperature, and means the higher flame height the bigger strength at the boarders. However according to Du (2000), the chemical reaction models affects the velocity very softly. The quasi global model was able to predict almost perfectly this parameter, with highly precision and also could explain a mistaken data from the flame sheet model, which has a supposed recirculation at the start, Fig.7, with values under zero, mentioned by Tarhan and Selçuk (2003), since the experimental data and the most complex model do not show this event. Westbrook and Dryer (1981) says that the flame velocity for rich mixture are elevated and at atmospheric pressure, results of detailed mechanisms reactions matches with experimental data.

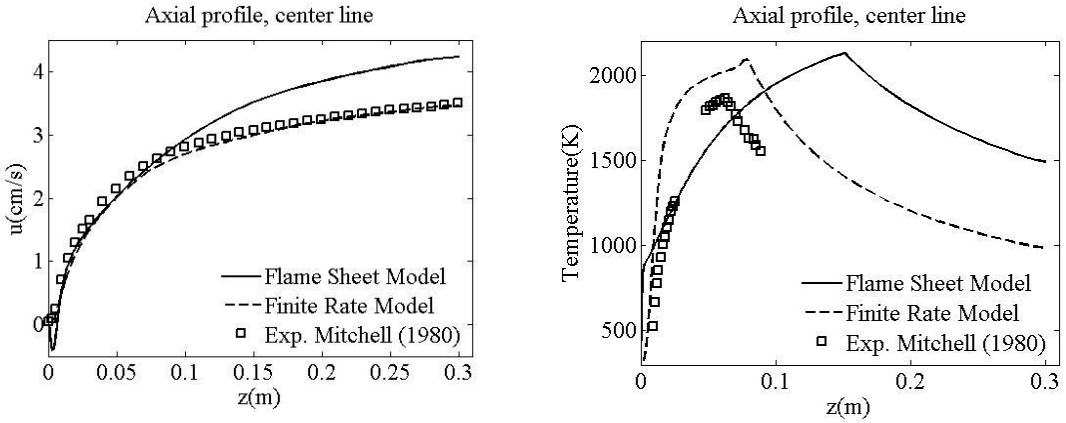


Figure 7. Axial centerline profiles of radical velocity component and temperature

According to other researches, Westbrook and Dryer (1981) concluded about the activation energy and it does not influences the methane, as well as, other n paraffinic fuels, since the flame velocity, pressure and variation rate was almost the same.

Assuming the CO_2 and H_2O as the only products of combustion, the total heat is overrated. The temperature (~2000 K) for adiabatic flames of typical hydrocarbons assumes that CO e H_2 are equilibrated with other combustion products. This is also true for less complex processes with another free radical species, for example H, O and OH. This equilibrium decreases the reaction heat and the adiabatic temperature below the expected values. This is clearly visible in Fig. 8, Westbrook and Dryer (1981).

It is known that burned gas contains CO e H_2 incompletely oxidized, and the typical hydrocarbons burn in a sequential way, this means that, the fuel is partially oxidized so are the CO and H_2, which still not all consumed until the hydrocarbons species have disappeared. Adding those two species with another improvement for many steps mechanisms causes temperature and composition to be more accurate, and save processing time Westbrook and Dryer (1981).

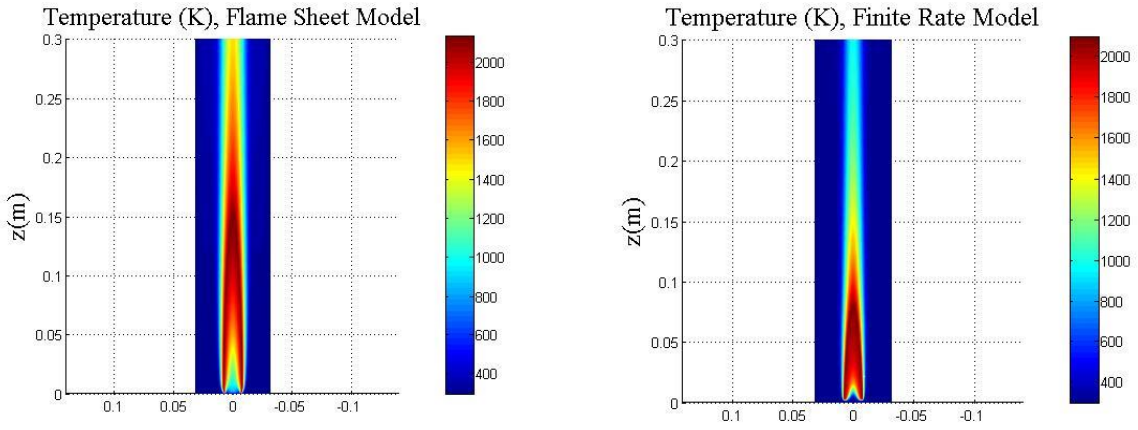


Figure 8. Temperature fields at steady state.

The temperature profile for the axisymmetric axis is much higher than the experimental data. The maximum flame height characterized by the highest temperature found in the experimental analysis was 5.8 cm by Mitchell *et al.* (1980) and 12 cm by Tarhan and Selçuk (2003). According to Fig. 8 the flame sheet model gives 15 cm as result, which is far from the reality and the quasi global gives 7.5 cm, in another words, an optimum result. Mitchell et al. (1980) also predict that numeric simulation always brings higher values of temperature, inside and outside the flame.

In Uygur's (2006) simulation considering radiation heat transfer for the same situation (single step reaction), the temperature value reaches close value to the experimental data. Some species as CO_2 and H_2O, which are the relevants for the heat transfer (both absorbs this emission), however do not show such difference in results due to moles fraction, which are more sensitive to those simulation mechanisms instead of temperature fields applied.

As soon as the flow begins, immediately starts the reaction and the high temperature region, which reaches the inlet until the axisymmetric axis. As it flows, the temperature field expands itself following the walls due to recirculation. In the farthest region the temperature drops, because of the conversion of the reactants into products. The final flame ends up in steady state after 2 seconds, shown in Fig. 8, with highly temperature gradients. Around the inlet, the temperature

rises from 298 K to 2000k in less than 1 cm. In the radical direction, is observed its decreasing and reaches the inlet value. The same result was found by Tarhan and Selçuk (2003).

4. CONCLUSIONS

The modelling and simulation of a non premixed combustion was presented in this work. Therefore, two models, flame sheet and finite rate were presented and discussed.

Simulated results from methane flame were very consistent with experimental data. For the flame sheet model, it was observed physics inconsistency, as the negative values from the velocity profile due to reflux, however all the divergences were already expected because of the flame sheet approximation

For the finite rate model the results showed much better accuracy, especially for velocity axial centerline profiles and peak temperature value, which considering the few chemical reactions simulated, was very close from real data.

It is known to get even better results and higher accuracy, more steps, chemical reactions and finer mesh should be added in the process or even radiation heat transfer for species such as CO_2 and H_2O, with the cost of much more processing time and considering for which purpose it will be applied. Time spent on processing the finite rate model was almost 13.5 times more than flame sheet model, it clearly means that flame sheet model for engineering applications is a very good option, despite that, for a scientific purpose would be better using the finite rate chemistry model with better accuracy and more details about much more chemical species.

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