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Obiettivo 5

Development of a Partially Premixed Combustion Model

by:

M. Talice and M. Mulas
Fluidynamics and Combustion Area
mulas@crs4.it, talice@crs4.it

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1 Introduction

A premixed combustion flow is characterized by a complete mixing of fuel (reactants) and oxidizer that exists before entering the combustion chamber, so that not only the mixture is ready to burn, but it is also characterized by uniform profiles of reactant's concentrations. This assumption can be actually considered true from an average point of view. Premixed theory, even if applicable to some cases of practical industrial interest, is somehow still far from being able to describe combustion in correct physical terms. When a premixed flame structure occurs is very likely that one of the following phenomena occurs:

- a complete turbulent mixing, but still incomplete molecular mixing (i.e. the profiles of average reactant's mixture concentrations are uniform, but pulsation of reactant mixture concentrations occur);
- non-uniform profiles of reactant's concentration in lean or in rich premixed flows (i.e. premixed combustion in flows with non-uniform distribution of the air excess coefficient);
- the presence of zones of lean and rich mixture composition with non-uniform profile of reactant's concentration, at different parts of the flow (i.e. the combustion process contains elements both of premixed and non-premixed combustion mechanism).

When dealing with real combustors, some of the above phenomena allways occur. When a more detailed and accurate description of combustion is needed, premixed combustion modeling has to be replaced with some "new modeling" capable to account for more detailed and complex physics involved. In the next sections a possible approach to model partially (or imperfectly) premixed combustion will be presented and its implementation into a CFD code will be illustrated. Finally, some preliminary results will be presented.

2 Premixed Combustion Basic Equations

Premixed turbulent combustion can be studied by following a pdf approach for a single thermochemical variable. The Bray-Moss-Libby theory [1], assuming unit Lewis number and one step chemistry, introduces a progress variable:

$$c = \frac{T - T_b}{T_u - T_b} \qquad\qquad c = \begin{cases} 0 \Rightarrow 100\,\%\,\text{reactants;} \\ \\ 1 \Rightarrow 100\,\%\,\text{products;} \end{cases}$$

where the suffixes b and u refer to burned and unburned mixture respectively. The equation for the progress variable c writes:

$$\partial\,(\overline{\rho}\,\widetilde{c})/\partial t + \nabla\cdot(\overline{\rho}\,\widetilde{c}\,\widetilde{\mathbf{u}}) = \nabla\cdot(-\overline{\rho\mathbf{u}''c''}) + \overline{W} \tag{1}$$

where $\overline{W}$ is the real chemical source term and $\nabla\cdot(-\overline{\rho\mathbf{u}''c''})$ is the turbulent transport term. It has to be noted that both these terms need closure models. By assuming that the pdf of the progress variable can be represented as given by two Dirac [2], located in correspondence of pure reactants and products, the problem is closed. In this approach, the progress variable is linked to mass density and temperature by the following algebraic relations:

$$\overline{\rho} = [\,(1-\widetilde{c})/\rho_u + \widetilde{c}/\rho_b\,]^{-1} \qquad \overline{T} = (1-\widetilde{c})\,T_u + \widetilde{c}\,T_b \tag{2}$$

It has been experimentally and theoretically demonstrated that a "counter-gradient" nature of the term $-\overline{\rho\mathbf{u}''c''} \equiv -\overline{\rho}\widetilde{\mathbf{u}''c''}$ exists, so that in order to describe it in terms of an effective diffusion coefficient, this coefficient can be negative. In fact, in this case the term containing the progress variable fluctuations can be expressed in terms of the average progress variable. Therefore, in a general approach, it cannot be modeled with the usual diffusion closure (the eddy viscosity closure):

$$-\overline{\rho}\widetilde{\mathbf{u}''c''} = D_t\nabla\widetilde{c}$$

unless a negative , and therefore unphysical, diffusion coefficient D_t is assumed. It has to be noted that, if conventional diffusion closure were applicable, the turbulent transport closure would have been achieved in terms of the average progress variable. Unfortunately, this is not the general case. Usually a second order closure has to be applied by involving the solution of a set of equations for the turbulent fluctuations $\widetilde{u''c''}$ [3].

2.0.1 The TFC closure: $1D$ case

The TFC model gives a closure of Eq. (1) by providing an expression for the two terms on the RHS: the turbulent transport term $\nabla \cdot (-\overline{\rho u'' c''})$ and the source term $\overline{W}$.

The closure procedure can be illustrated starting from a one-dimensional case. Equation (1) for a 1D case reads:

$$\frac{\partial(\overline{\rho}\,\tilde{c})}{\partial t} + \frac{\partial(\overline{\rho}\,\tilde{u}\,\tilde{c})}{\partial x} = \frac{\partial(-\overline{\rho}\,\widetilde{u''\,c''})}{\partial x} + \overline{W} \tag{3}$$

In a frame of reference moving with the turbulent flame speed U_t ($x' = x - U_t \cdot t$, and $t' = t$) equation (3) becomes:

$$\overline{\rho}\,\frac{\partial\tilde{c}}{\partial t'} + \rho_u\,U_t\,\frac{\partial\tilde{c}}{\partial x'} = -\frac{\partial(\overline{\rho}\,\widetilde{u''\,c''})}{\partial x'} + \overline{W} \tag{4}$$

with $\overline{\rho}\,\tilde{u} = \rho_u\,U_t = const$ for mass conservation.

As discussed in [4], for $t \ll \tau_{st}$ (ISP flames) the turbulent flame brush will increase its thickness with time according to the turbulent dispersion law. A modelling equation for such a front is then:

$$\overline{\rho}\,\frac{\partial\tilde{c}}{\partial t'} = \frac{\partial}{\partial x'}\left[\overline{\rho}\,D_t\frac{\partial\tilde{c}}{\partial x'}\right], \tag{5}$$

where D_t is the turbulent diffusion coefficient.

By using this expression in equation (4) it can be obtained:

$$\rho_u\,U_t\,\frac{\partial\tilde{c}}{\partial x'} = \overline{W} + \frac{\partial}{\partial x'}\left[-\overline{\rho}\,\widetilde{u''\,c''} - \overline{\rho}\,D_t\frac{\partial\tilde{c}}{\partial x'}\right] \tag{6}$$

which shows that the term on the L.H.S. may be used to model the progress variable source term $\overline{W}$ and the difference between the second order velocity-progress variable correlation and the actual turbulent transport term.

At this point an estimation for the average source term in Eq. (6) has to be set. It is assumed to be proportional to the probability to find the flamelet at a given position $p_{flam}(x,t)$; this probability is related to the probability of finding products P_b at the given position by the relation:

$$P_b(x,t) = \int_{-\infty}^{x} p_{flam}(x,t)\,dx \quad \Rightarrow \quad p_{flam}(x,t) = \frac{\partial P_b}{\partial x} \tag{7}$$

It has also to be noted that

$$\overline{c} = P_b\,1 + (1 - P_b)\,0 = P_b \tag{8}$$

Therefore we can write:

$$\overline{W} = const\,\frac{\partial \overline{c}}{\partial x'} \qquad\qquad \overline{W} = \rho_u\,U_t\,\frac{\partial \overline{c}}{\partial x'} \tag{9}$$

where the result $const = \rho_u\,U_t$ can be shown by integrating equation (6) from $-\infty$ to $+\infty$.

By using Eq. (9) in Eq. (6) the following expression for the space derivative of the second order velocity-progress variable correlation is obtained:

$$-\frac{\partial(\overline{\rho}\,\widetilde{u''\,c''})}{\partial x'} = \rho_u\,U_t\,\frac{\partial(\tilde{c}-\overline{c})}{\partial x'} + \frac{\partial}{\partial x'}\left[\overline{\rho}\,D_t\frac{\partial\tilde{c}}{\partial x'}\right] \tag{10}$$

By using Eqs. (9) and (10) into Eq. (4):

$$\overline{\rho}\,\frac{\partial\tilde{c}}{\partial t'} + \rho_u\,U_t\,\frac{\partial\tilde{c}}{\partial x'} = \frac{\partial}{\partial x'}\left[\overline{\rho}\,D_t\frac{\partial\tilde{c}}{\partial x'}\right] + \rho_u\,U_t\,\frac{\partial\overline{c}}{\partial x'}$$

and now passing to the fixed frame of reference the final TFC closure for the 1D case it is achieved:

$$\frac{\partial(\overline{\rho}\,\tilde{c})}{\partial t} + \frac{\partial(\overline{\rho}\,\tilde{u}\,\tilde{c})}{\partial x} = \frac{\partial}{\partial x}\left(\overline{\rho}\,D_t\,\frac{\partial\tilde{c}}{\partial x}\right) + \rho_u\,U_t\,\left|\frac{\partial\tilde{c}}{\partial x}\right| \tag{11}$$

where D_t is the physical positive turbulent diffusion coefficient, and U_t is the turbulent combustion velocity. The absolute value in the source term is a generalization that makes possible to account for a positive definite U_t for flames traveling in both directions (x and $-x$).

2.0.2 TFC Closure Equation: $3D$ formulation

The TFC model for the general 3d case requires to solve an equation for the progress variable $\tilde{c}$ in the form of:

$$\partial\,(\overline{\rho}\,\tilde{c})/\partial t + \nabla\cdot(\overline{\rho}\,\tilde{c}\,\tilde{\mathbf{u}}) = \nabla\cdot(\overline{\rho}D_t\nabla\tilde{c}) + \rho_u\,U_t\,|\nabla\tilde{c}| \tag{12}$$

To close Eq. (12) express U_t must be expressed as a function of the physico-chemical properties of the combustible mixture and turbulence parameters. In 1-D case U_t is the turbulent combustion velocity $U_t = U_f\overline{(S/S_0)}$. It can be defined under the assumption of fast chemistry ($\tau_{ch} \ll \tau_t$) and by modeling micro-turbulence and molecular transfer processes. But, if equilibrium of fine scale vortices and of small scale wrinkled flamelet sheet is assumed, the controlling parameters of the combustion model will be reduced to the molecular transfer coefficient χ, the chemical time $\tau_{ch} = \chi/U_L^2$ and the integral turbulent characteristics $u' = \sqrt{\overline{u'^2}}$ and l_t.

2.0.3 Turbulent Flame Velocity

In TFC approach [2] the Turbulent Flame Velocity is modeled as:

$$U_t = A\,G\,u'^{3/4}\,U_l^{1/2}\,\chi^{-1/4}\,l_t^{1/4} \tag{13}$$

where:

U_l	laminar flame velocity	mixture property
χ	molecular heat transfer coefficient	mixture property
u'	RMS (root-mean-square) of velocity fluctuations	$\sqrt{\frac{2}{3}\kappa}$
l_t	turbulence lenght scale	$C_D\frac{u'^3}{\epsilon}$
κ	turbulent kinetic energy	computed from turbulence model
ϵ	turbulent kinetic energy diddipation	computed from turbulence model
G	stretch factor	
C_D	model constant	0.37
A	model constant	0.52

The stretch factor G can be modeled as follows:

$$G = \frac{1}{2}\left[1 + z_{nnn}\left[1 - c_1 sp_2 - c_2 {sp_2}^2 + c_3 {sp_2}^3\right] e^{-{sp_1}^2}\right] \tag{14}$$

$$sp_1 = \frac{\frac{\sigma}{2} + \log dcr}{\sqrt{2\sigma}} \qquad sp_2 = \frac{1}{1 + c_4 sp_1 z_{nnn}}$$

$$dcr = \frac{15\nu gcr^2}{\epsilon} \qquad \sigma = \delta \log\left[\left(\frac{u' l_t}{\nu}\right)^{3/4}\right]$$

with:

$$z_{nnn} = +1 \qquad if\,sp_1 \geq 0; \qquad z_{nnn} = -1 \qquad if\,sp_1 \leq 0$$

Values for the constants c_1, c_2, c_3, c_4 and δ are as follows:

$$\begin{aligned} c_1 &= 0.34880242 \\ c_2 &= 0.0958709 \\ c_3 &= 0.7478556 \\ c_4 &= 0.47047 \\ \delta &= 0.26 \end{aligned}$$

3 Partially (or Imperfectly) Premixed Modeling

3.1 Generality

Three possible combustion regimes are schematically represented in figure 1.

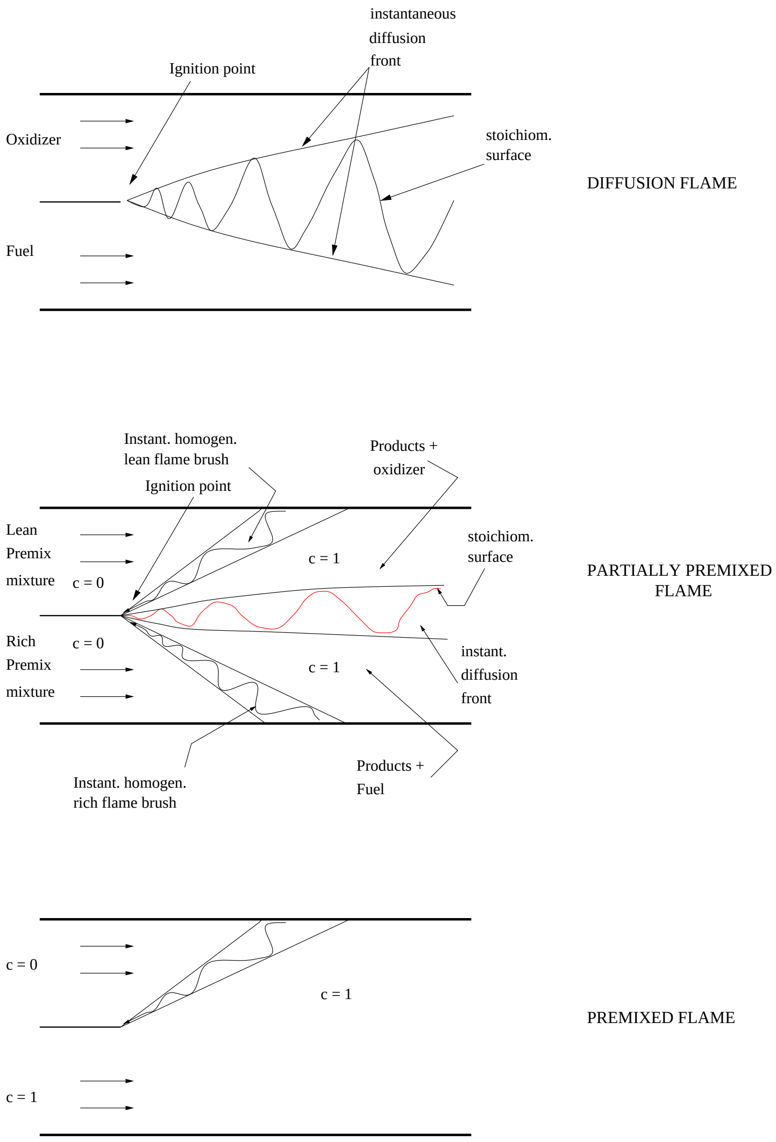

Figure 1: Three possible flame's topology

1. At the top part of figure 1, a pure diffusive flame is shown. Two separated streams of fuel and oxidizer enter the combustor with given composition, tem-

perature and pressure. Combustion starts at the ignition point and it is sustained by molecular and turbulent mixing.

2. At the bottom part of the same figure 1, the perfectly premixed case is illustrated. A burned stream of gas is used to stabilize the combustion of a perfectly premixed mixture of fuel and oxidizer. The value of the progress variable c at several locations is indicated in the figure. According to its previously discussed meaning, $c = 0$ means uncombusted mixture, whereas $c = 1$ occurs in correspondence of complete combustion. As it can be seen from figure 1 the gas is completelly burned behind the flame front.

3. At the middle part of figure 1 a possible situation of partially premixed combustion is shown. Two streams of rich and lean premixed mixture feed the combustor from the upper and lower injection ducts. It has to be remembered here that lean mixture means that the fuel mass fraction in the mixture is less than its stoichiometric value, so that downstream the premixed flame brush, some oxidizer is left. On the other hand, in the rich case, the combustion products still contain some extra fuel, for the oxidizer is not enough to burn all the fuel in the mixture. Thus, downstream the two premixed flame brushes on the lean and rich sides ($c = 1$ zone), two streams of fuel and oxidizer will be available to be burned according to a diffusion like combustion process.

A simpler case of partially premixed combustion, but still important for many indistrial applications, occurs when the combustor is fed by two streams of both rich or lean mixtures, but with different value of the mixture fraction. A third stream of burned gas is used in order to stabilize the flame. The phisical model is sketched in figure 2. In this case there is no possibility for the existence of any diffusion flame behind the premixed flame brushes, for the exhaust gas will be short of oxidizer or fuel, respectivelly. Nevertheless, this is still a quite interesting situation, because in the actual industrial burners it is unlike to have perfectly controlled premixed mixtures, the composition of which being non uniform and non constant in space and in time.

In the following the term *partially premixed* will refer to the case described in the middle part of figure 1, whereas by *imperfectly premixed* will be meant the situation shown in firgure 2. Through the next chapters a possible way to model the imperfectly premixed case will be illustrated. Finally, a brief description of how to get a closure for a more general partially premixed model will be given.

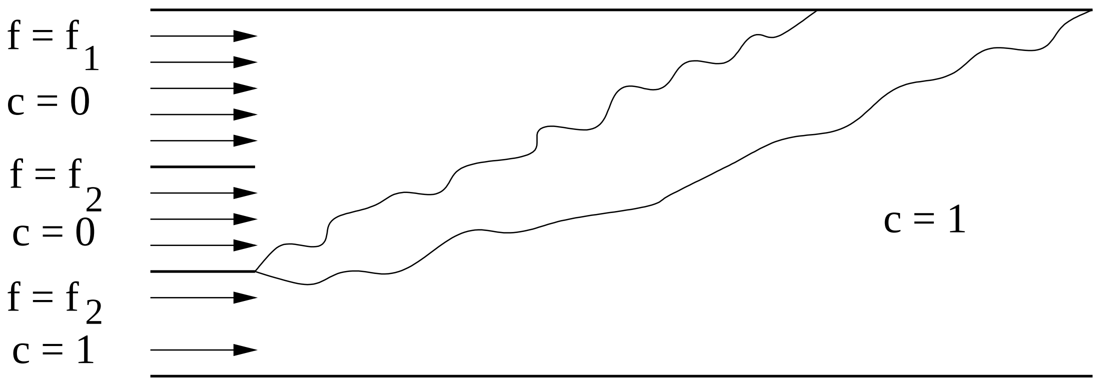

Figure 2: The model case

3.2 Imperfectly Premixed Model IPM

In order to attempt a suitable modeling of the imperfectly premixed combustion process, the idea was to start from the TFC formulation and to extend the model to the partially (or imperfectly) premixed case, with the limitation already discussed. In the case under consideration, the mixture properties cannot be considered uniform and constant anymore. In particular, the laminar flame velocity S_L and the molecular heat transfer coefficient χ, do assume different values in dependence on the spatial properties of the mixture itself. Both S_L and χ are then to be considered function of some mixture property, such as the mixture fraction f or the corresponding equivalence ratio ϕ, that would be suitable to describe the mixture's composition at any point and at any time. Therefore the only TFC's equation for the progress variable $\tilde{c}$ is not enough anymore and a new equation has to be solved in order to know the value of f in space and time. In other words, the TFC approach is still valid, but on a local scale, only.

3.2.1 An Equation for the Mixture Fraction

The mixture fraction **f** is a normalized fraction of the fuel to oxidizer ratio at each control volume, ranging from 0 to 1. A simple way to derive the mixture fraction **f**, starts from considering the generic combustion equation:

$$fuel \quad + \quad sOx \quad \rightarrow \quad (1+s)\, products \tag{15}$$

where **s** is stoichiometric oxidizer concentration. If the mass fraction is defined as:

$$\psi = m_{fu} - \frac{m_{ox}}{s}$$

the (15) can be re-written in terms of ψ and the mixture fraction **f**, as follows:

$$\psi_{fuel} \quad + \quad (1 - \mathbf{f})\, \psi_{\text{inf}} \quad = \quad \psi \tag{16}$$

in which:

$$\psi_{fuel} \quad = mass\, fraction\, of\, fuel\, in\, the\, fuel\, stream$$

and

$$\psi_{\text{inf}} \;=\; mass\, fraction\, of\; oxydizer\; in\; ambient\; air$$

Solving equation (16) for **f** leads to the definition of the mixture fraction **f**:

$$\mathbf{f} \equiv \frac{\psi - \psi_{\text{inf}}}{\psi_{fuel} - \psi_{\text{inf}}} \tag{17}$$

If $\mathbf{f} = 0$ the mixture contains only ambient oxidizer concentration; if $\mathbf{f} = 1$ the mixture contains pure fuel. In stoichiometric condition it is:

$$\mathbf{f}_{\text{st}} = \frac{\psi_{\text{inf}}}{\psi_{fuel} + \psi_{\text{inf}}} \tag{18}$$

The mixture fraction **f** is a conserved scalar (i.e. there is no a source term in the transport equation for **f**), and such transport equation can be written as:

$$\partial\,(\overline{\rho}\,\widetilde{f})/\partial t + \nabla \cdot \left(\overline{\rho}\,\widetilde{f}\,\widetilde{\mathbf{u}}\right) = \nabla \cdot (\overline{\rho} D_t \nabla \widetilde{f}) \tag{19}$$

in which:

D_t the turbulent diffusion coefficient, given by:

$$D_t = \frac{\nu_t}{\sigma_t}$$

with: σ_t is the turbulent Prandtl number.

Beside **f** the equivalence ration can also be defined as:

$$\phi = \frac{f}{1 - f}\,\frac{1 - f_s t}{f_s t} \tag{20}$$

3.2.2 The Proposed Imperfectly Premixed Model Equations

The Imperfectly Premixed Model couples the TFC equation for the progress variable $\tilde{c}$ with the transport equation for **f**, thus:

$$\begin{aligned} &\partial\,(\overline{\rho}\,\tilde{c})/\partial t + \nabla\cdot(\overline{\rho}\,\tilde{c}\,\tilde{\mathbf{u}}) = \nabla\cdot(\overline{\rho}D_t\nabla\tilde{c}) + \rho_u\,U_t\,|\nabla\tilde{c}| \\ &\partial\,(\overline{\rho}\,\tilde{f})/\partial t + \nabla\cdot\left(\overline{\rho}\,\tilde{f}\,\tilde{\mathbf{u}}\right) = \nabla\cdot(\overline{\rho}D_t\nabla\tilde{f}) \end{aligned} \tag{21}$$

The turbulent flame velocity can be still expressed, as previously done for the TFC model, as:

$$U_t(f) = A\,G\,u'^{3/4}\,S_L(f)^{1/2}\,\chi(f)^{-1/4}\,l_t^{\,1/4} \tag{22}$$

where it can be noted that the laminar flame velocity S_L and the molecular heat transfer coefficient χ are now functions of the mixture fraction **f**. Furthermore, a short comment on how to evaluate the temperature $\tilde{T}$ and density $\overline{\rho}$, has to be made at this stage. In rigorous terms, values for $\tilde{T}$ can be computed as:

$$\tilde{T} = \tilde{c}\int T_{ad}(f)\,P(f)\,df + (1-\tilde{c})\int T_u(f)\,P(f)\,df \tag{23}$$

because we assume that $T_u(f) = T_u = const$ for given conditions, the 23 can be rewritten as:

$$\tilde{T} = \tilde{c}\int_0^1 T_{ad}(f)\,P(f)\,df + (1-\tilde{c})\;T_u\int_0^1 P(f)\,df \tag{24}$$

but: $\int_0^1 P(f)\,df = 1$, then:

$$\tilde{T} = \tilde{c}\int_0^1 T_{ad}(f)\,P(f)\,df + (1-\tilde{c})\;T_u \tag{25}$$

by assuming a Dirac like distribution for the probability function $P(f)$, the (25) reduces to:

$$\tilde{T} = T_u + \tilde{c}\,(T_{ad}(f) - T_u) \tag{26}$$

by following the same approach, an expression for $\overline{\rho}$ can also be found:

$$\overline{\rho} = \frac{1}{\frac{(1-\tilde{c})}{\rho_u(f)} + \frac{\tilde{c}}{\rho_b(f)}} \tag{27}$$

In order to be able to close the model, it has to be known how to deal with the following:

$$S_L = S_L(f); \quad \chi = \chi(f); \quad T_{ad} = T_{ad}(f); \quad \rho_u = \rho_u(f) \quad and \quad \rho_b = \rho_b(f)$$

This will be briefly discussed through the next paragraps.

3.3 Factors Influencing Laminar Flame Velocity

Many factors influence the laminar flame speed, namely temperature, pressure, equivalence ratio and fuel type. In [5] a detailed analysis of these dependencies can be found. Hereafter a short summary will be reported.

3.3.1 Temperature

Dependency of laminar flame speed on temperature can be expressed as follows:

$$S_L \propto \bar{T}^{-0.5} {T_u}^{0.5} {T_b}^{-n/2} \exp\left(-E_A/2R_u T_b\right) P^{(n-2)/2} \tag{28}$$

where it is:

$$\bar{T} = 0.5 * (T_u + T_b)$$

Since the global reaction order **n** for hydrocarbons is about two and the apparent activation energy is approximately $1.67x10^8$ J/kmol, from equation 28 it appares that the laminar flame speed has a quite strong dependence on the temperature of the unburned mixture. For example, by applying equation 28, the flame speed is seen to be increased by a factor of 2.89 when the unburned gas temperature is increased from 300 K to 600 K. Some empirical correlations to estimate the influence of temperature on flame speed can be found in [6] and [7].

3.3.2 Pressure

Equation 28 shows a dependence of laminar flame speed on pressure of the type:

$$S_L \propto P^{(n-2)/2} \tag{29}$$

In the case of hydrocarbon fuels it has been already tested that the global reaction order **n** is approximately equal to two, so that S_L should be independent on pressure. Experimental measurements generally show a negative dependence on pressure. However, this effect is much less significant than dependence on temperature.

3.3.3 Equivalence Ratio

Except for very rich mixtures, the primary effect of equivalence ratio on the flame speed is a results of how this parameters influences the flame temperature. Thus, for a given T_u of the unburned mixture, higher values of the reaction products temperature T_b correspond to growing values of the equivalence ratio ϕ. As a consequence, by application of equation 28 it can be seen that also S_L will be increased.

3.3.4 Fuel Type

A few collections of flame speed measurements for different fuels are available in literature. Among them some of the more realiable are those by [8] and by [9].

3.3.5 Flame Speed Correlations

In [7] several regression formula have been tested in order to correlate the laminar flame speed of various fuel-air mixture to a range of temperatures and pressures typical of realistic operative conditions. One of the most promising formula is of the form:

$$S_L = S_{L,ref}\left(\frac{T_u}{T_{u,ref}}\right)^{\gamma}\left(\frac{P}{P_{ref}}\right)^{\beta} \tag{30}$$

where is:

$$\begin{aligned} T_{ref} &= 298\ [\mathrm{K}] \\ P_{ref} &= 1\ [\mathrm{atm}] \\ S_{L,ref} &= B_M + B_2\,(\phi - 1.08)^2 \\ \gamma &= 2.18 - 0.8\,(\phi - 1) \\ \beta &= -0.16 + 0.22\,(\phi - 1) \end{aligned}$$

B_M, B_2, γ and β are correlation coefficients that have to be determined both from some data collections or from a pre-processor stage.

3.4 Factors Influencing the Molecular Heat Transfer Coefficient

Dependency of the molecular heat transfer coefficient is essentially on pressure and can be evaluated as follows:

$$\chi(\phi) = \frac{\chi_{ref}(\phi)}{P} \tag{31}$$

where $\chi_{ref}(\phi)$ is the value at $P = 1$ [atm] and pressure P must be expressed in [atm].

3.5 An example: Methane-Air Mixture

Hereafter, S_L and anything else needed to apply the proposed imperfectly premixed model, will be determined in the case of a mixture of methane (CH_4) and air. For the sake of generality and because quite often data collections are not easy to be found, mixture properties have been determined by using the Chemkin Collection Package, and its Premix application in particular. The Premix application allows for computing laminar flame speed, temperature, density and species mole fraction of a mixture of given equivalence ratio ϕ. By repeating the computation with several values of ϕ, it has been possible to get a set of discrete data and to determine the unknown coefficients in the correlation formula 30. Moreover, linear, quadratic and cubic interpolation formula have been applied to the computed values of ρ_u, ρ_b and T_b.
Relations 32, 33, 34 and 35 summarize the obtained results. By starting from equation 35 and by applying equation 30, the actual value of the laminar flame speed can be computed. Figures 3, 4, 5, 6 and 7 represent the above relations in graphical form. It must be reminded here that the burned gas temperature T_b is not used by the model. Nevertheless, the form of function 34 is important to be known at post-processing stage in order to compute the actual temperature at any point inside the combustion chamber, by application of equation 26

Finally, it has to be reminded here that all the previously reported relations are obtained by interpolation of a discrete set of data, thus all of them are valid for a restricted range of values of the mixture equivalence ratio ϕ. The arbitrary use of such expressions outside the range of validity, could lead to unphysical results. In the present case, the range of ϕ for which relations from 32 to 35 are defined was $0.8 \leq \phi \leq 1.1$.

$$\rho_u(\phi) = 0.607794 - 0.05763\phi \tag{32}$$

$$\rho_b(\phi) = 0.4901 - 0.629\phi + 0.2888\phi^2 \tag{33}$$

$$T_b(\phi) = 1.619E04 - 4.77E04\phi + 5.294E04\phi^2 - 1.921E04\phi^3 \tag{34}$$

$$S_{L,ref}(\phi) = 33.94 - 191.378 * (\phi - 1.08)^2 \tag{35}$$

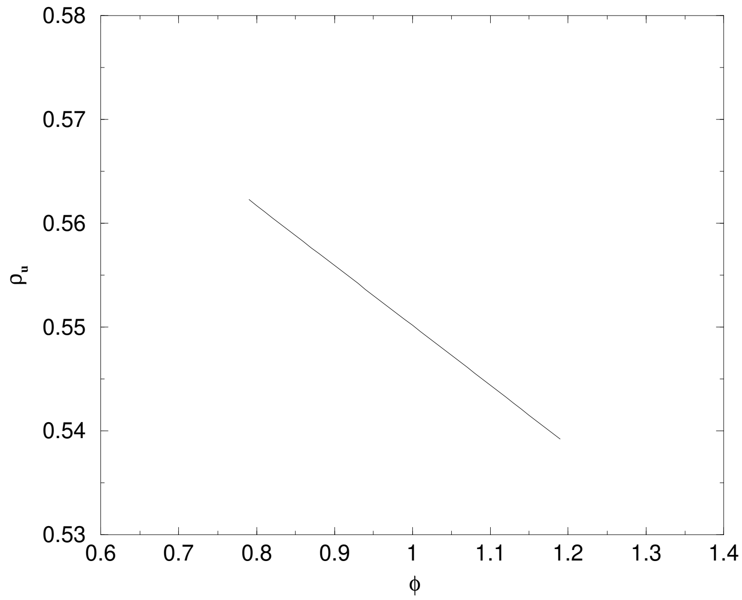

Figure 3: Density of unburned mixture as a function of ϕ

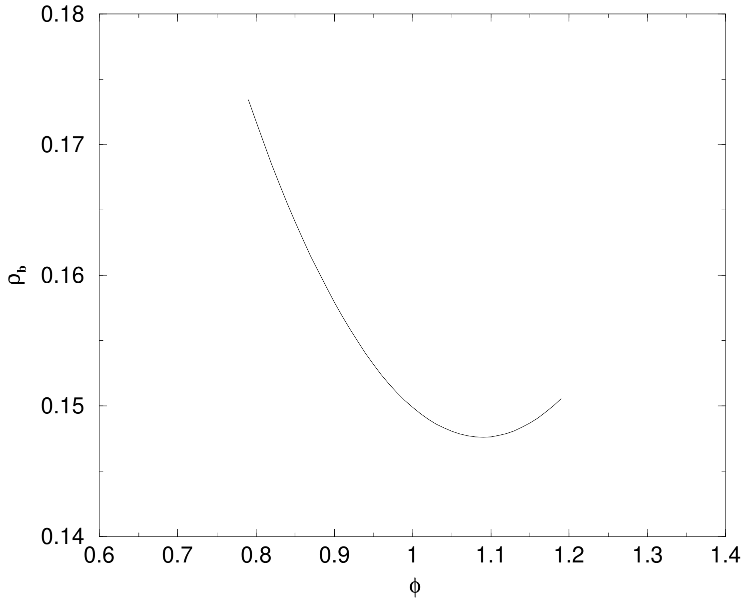

Figure 4: Density of burned mixture as a function of ϕ

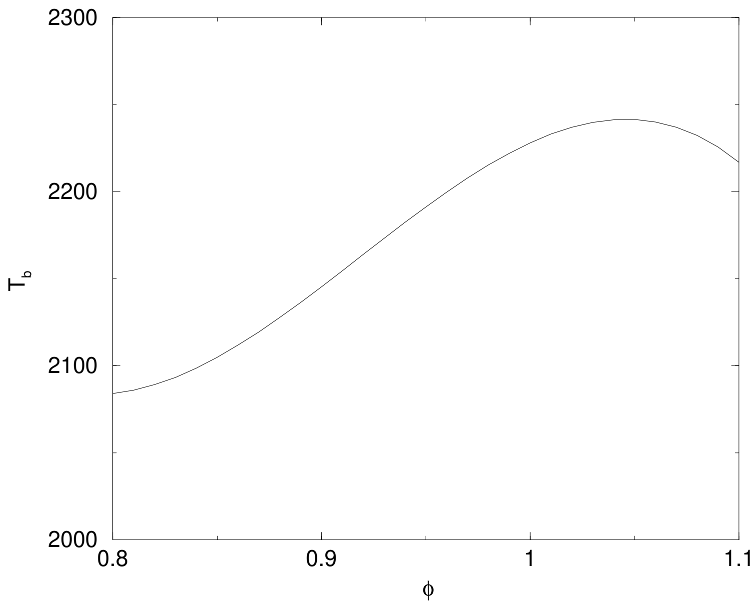

Figure 5: Temperature of burned mixture as a function of ϕ

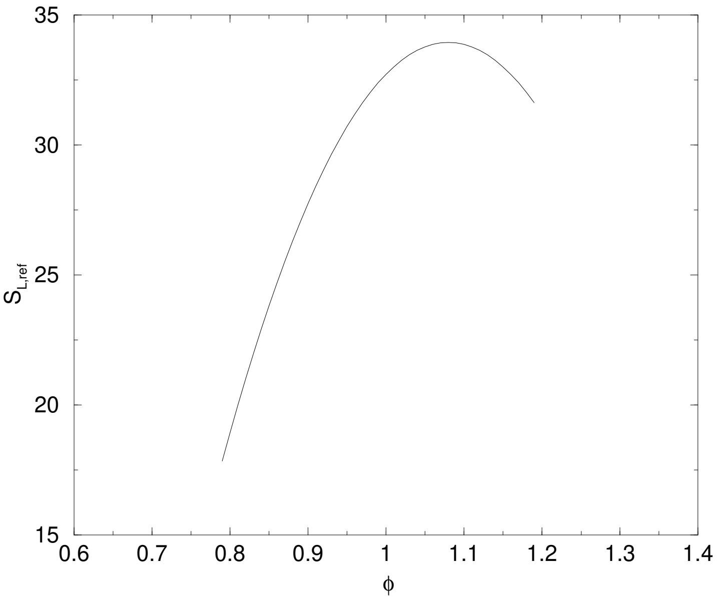

Figure 6: Reference Laminar Flame Speed as a function of ϕ

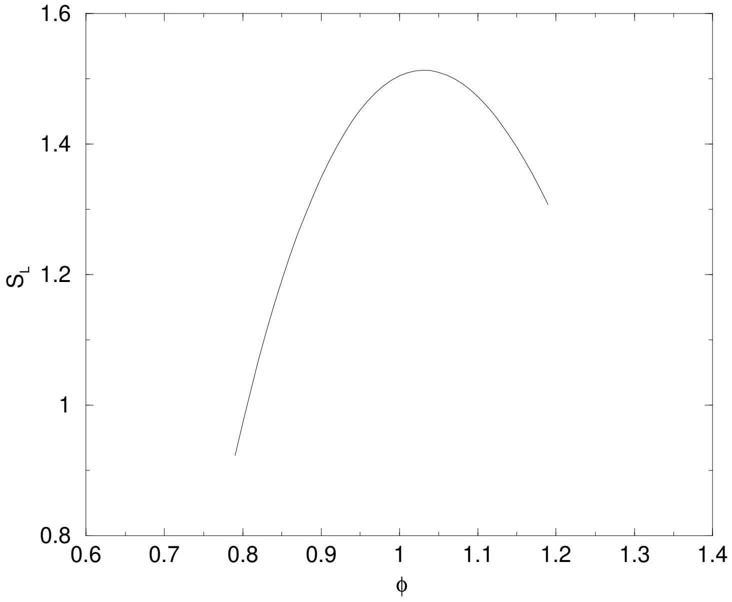

Figure 7: Laminar Flame Speed as a function of ϕ

3.6 Model's Assessment

The previously discussed imperfectly premixed model (hereafter referred to as IPM) has been initially validated against the standard TFC model. In fact, in the case of a mixture of constant ϕ, the equation for the mixture fraction $\mathbf{f}$ must be ineffective and the IPM model must reproduce the same results provided by the TFC model. The test case that has been chosen is the burner experimentally tested by Moreau [10]. The combustor geometry is shown in figure 8. The upper inlet has been split in two parts, so that it would be eventually possible to feed the combustor with fresh mixtures characterized by different values of ϕ. For the present experiment, however, the mixture (Methane and air) had the same composition at all the combustor's inlets. Part of the exhaust gas ($\tilde{c} = 1$) is recirculated and re-enters the combustor from the bottom duct. This stream is used to stabilize the flame. Flows properties are sumarized in table 1.

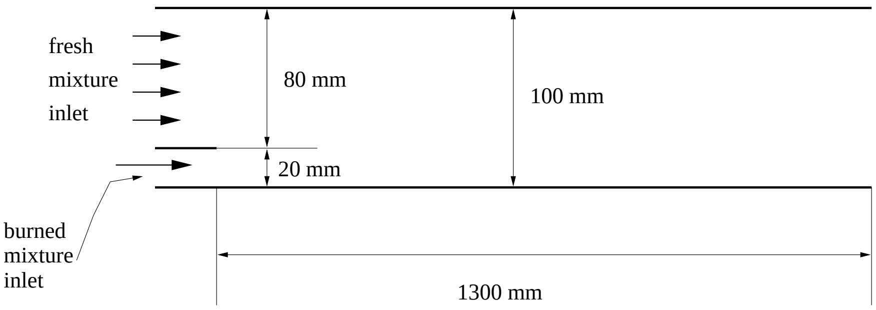

Figure 8: Combustor's geometry

	FRESH MXT.	BURNED MIXT.
Velocity [m/s]	65	116
Turbulence Intensity	0.012	0.021
Turbulencs Lenght Scale [m]	0.0056	0.0014
Progress Variable	0	1
Equivalence Ratio	0.84	0.84
Temperature [K]	600	2086

Table 1:

Laminar flame velocity, molecular heat transfer coefficient and all the other physical properties of interest have been evaluated by following the approach explained in previous sections. The used turbulence model was the Wilcox $\kappa - \omega$ two equation model re-written in $\kappa - log(\omega)$ form [11]. Figures 9 and 10 show the results obtained by using the TFC and the IPM models. As it can be seen, results are the same, as expected.

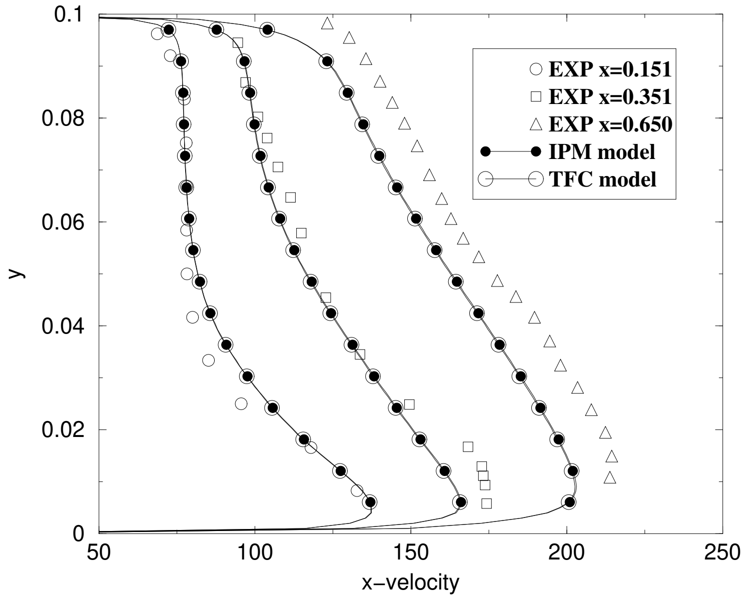

Figure 9: Velocity profiles at 151, 351 and 650 mm from inlet

The IPM model has been then tested from a qualitatively point of view only, by feeding the two upper inlets of the burner with mixtures of CH_4 and air characterized by different values of the equivalence ratio ϕ, namely $\phi = 0.84$ and $\phi = 1.0$ at the middle inlet section and at the top inlet section respectively. From the in-duct at the bottom of the combustion chamber a stream of exhaust gas ($\phi = 0.84$) has been used in order to stabilize the flame, as in the previously described case. Table 2 sumarizes the most significant test case features.

	FRESH MXT. TOP	FRESH MXT. MIDDLE	BURNED MXT. BOTTOM
Velocity [m/s]	65	65	116
Turbulence Intensity	0.012	0.012	0.021
Turbulencs Lenght Scale [m]	0.0056	0.0056	0.0014
Progress Variable	0	0	1
Equivalence Ratio	1.00	0.84	0.84

Table 2:

Figure 11 shows profiles of ϕ at 5 cross sections along the combustor. In the same figure inlet conditions for $\tilde{c}$ and ϕ are also indicated. From figure 11 it can be

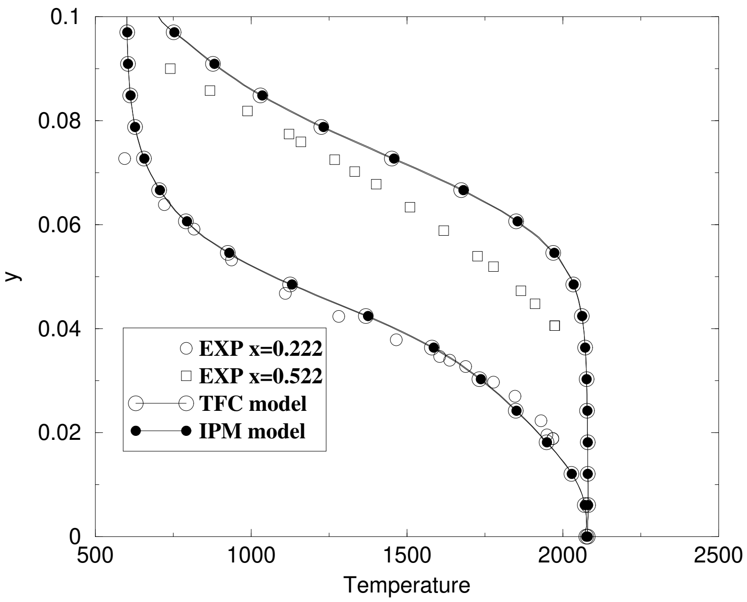

Figure 10: Temperature profiles at 222 and 622 mm from inlet

seen how the richer mixture is convected and diffused along the burner, according to equation 19.

In figure 12 the cross distribution of the laminar flame speed is represented at the same sections. It has to be reminded here that S_L is a given function of ϕ, as previously defined in equation 35. The previously described diffusion process of ϕ, gradually increases the value of S_L, moving downstream the chamber.

As a consequence the velocity and temperature profiles are different from the previous case of uniform mixture. This is shown in figures 13 and 14, respectively. Figure 14 shows that the combustion process is now more intense, as has to be expected for the mixture contains more fuel. At any point then, temperature is higher than in the constant ϕ case, and being the pressure almost constant, the effect of this higher temperature is to decrese the mixture density. According to the conservation of mass, velocity must then be higher at any section. This is in fact what appears in figure 13.

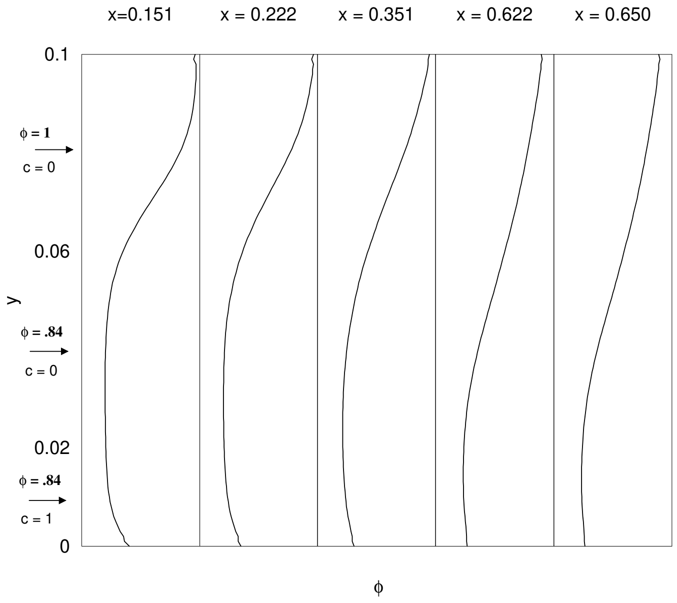

Figure 11: Equivalence ratio profiles at 151, 222, 351, 622 and 650 mm from inlet

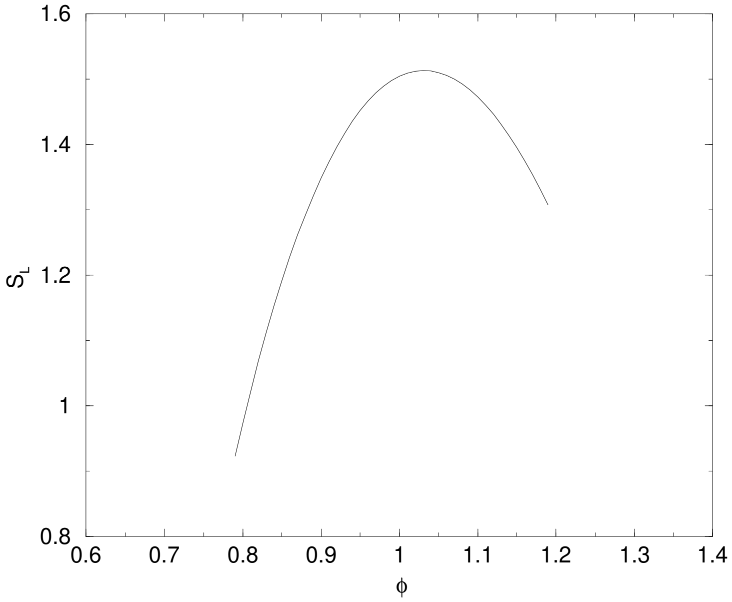

Figure 12: Laminar Flame Speed profiles at 151, 222, 351, 622 and 650 mm from inlet

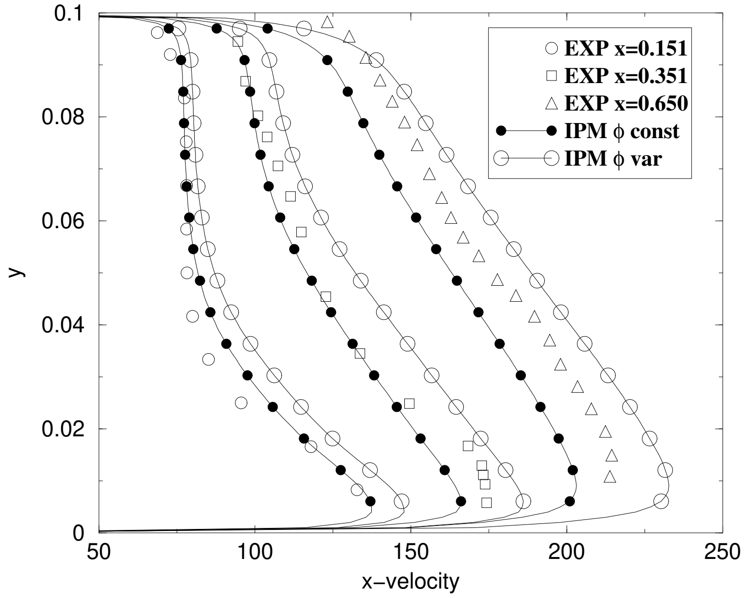

Figure 13: Velocity profiles at 151, 351 and 650 mm from inlet

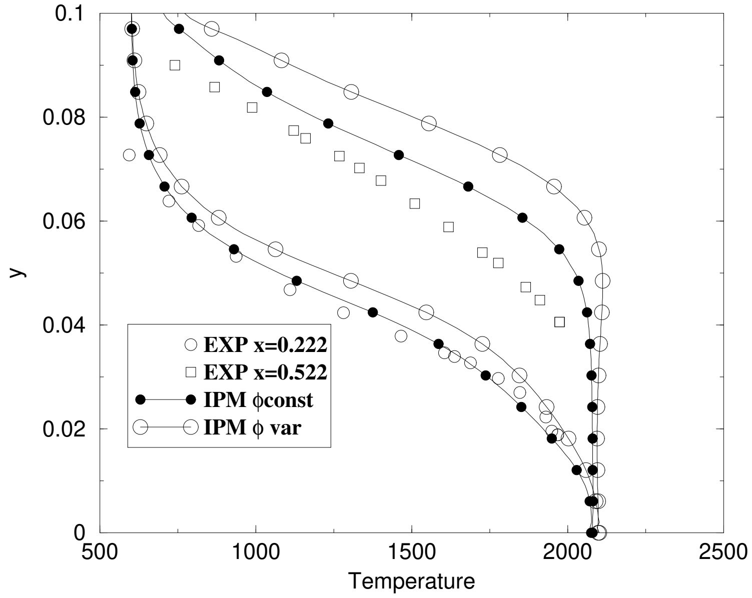

Figure 14: Temperature profiles at 222 and 622 mm from inlet

3.7 Extension to the Partially Premixed Case

With reference to the case already described in the middle section of figure 1, a possible modeling of the Partially Premixed Case will be briefly discussed. As a result of the premixed combustion process of the rich and lean mixtures that takes place in the first part of the combustion chamber, two streams of exhaust gas still containing fuel and oxidizer, respectivelly, are made available for a diffusion combustion process. The Partially Premixed Model then, should be somehow a combination of two main moments, namely a purely premixed model (or imperfectly one), followed by any suitable diffusion model.

Regardless to the actual type of process (premixed or diffusion), the goal of modeling combustion is to provide a suitable form of the equation of state, namely to define a proper linking among thermo-dynamic quantities. For example, in the case of the TFC or of the IPM model, under the given hypothesis of steady, incompressible and adiabatic flow, such equation os state has been written as:

$$\rho = \rho\left(\hat{c}, (f)\right)$$

Equations 2 and 27 provide the form of the equation of state explicitely. With reference again to figure 1, the same kind of modeling can be applied to the "premixed" part of the combustor. From the premixed brushes on, turbulent diffusion combustion takes place into the combustion chamber. Many different approaches to turbulent diffusion combustion modeling can be found in leterature (see for example [5], [12], [13], [14]). The most simple approach is to consider the existence of chemical equilibrium and to make use of an appropriate conserved scalar (i.e. the mixture fraction) in order to describe the flow composition at any point and at any time. Once the composition is known, the value of all the quantities of interest can be found. More sophisticated approaches, take into account the influence of pulsation in the composition of the mixture due to turbulence. A suitable approach is then to add to the equation for the conserved scalar, one extra equation for its variance, plus any appropriate probability density function to describe in statistical terms the pulsating phenomena. Whatever the chosen approach is, and whatever is the complication involved, the goal of the modeling is to provide again a suitable form for the equation of state, which is used to close the problem. In other words, the general form for the PPM equation of state could be expressed as:

$$\rho_{PPM} = \underbrace{\alpha\rho_{IPM}\left(t, \hat{c}, f\right)}_{\text{imperfectly premixed part}} + \underbrace{\left(1-\alpha\right)\rho_{diff}\left(f, \left(f', ...\right)\right)}_{\text{diffusion part}} \qquad (36)$$

in which α is a parameter that is set to one in the premixed zone and to zero behind.

4 Conclusions

In this work, a possible extension of the TFC model to imperfectly premixed cases has been introduced and validated, even if in a purely qualitative way. The proposed IPM model has given results phisically consistent and it seems able to describe in more correct terms actual combustor, in which it is far from real any assumption of having perfectly premixed mixtures feeding the combustion chamber. Nevertheless, a proper validation of the proposed IPM model and of the TFC model over a realistic industrial case is still to come and it will be an essential part of the future work. Finally, the quite general lines of how to get a partially premixed model (premixed plus diffusion) have been drawn, showing that, in principle, no new modeling is needed and that it would be probably enough to assembly already existent premixed and diffusion models. The actual implementation of the idea above into **ARES** could be also a future development of this work.

References

[1] Bray, K.N.C. "Turbulent Flows with Premixed Reactants". In Libby P.A. and Williams F.A., editors, *Turbulent Reacting Flows*, Topics In Applied Physics, Vol. 44, pages 115–183. Springer-Verlag, 1980.

[2] Zimont, V.L. Theory of Turbulent Combustion of a Homogeneous Fuel Mixture at High Reynolds Number. *Combustion, Explosion, and Shock Waves*, 15(3):305–311, Nov. 1979.

[3] Bailly, P., Champion, M., and Garréton, D. Counter-gradient diffusion in a confined turbulent premixed flame. *Physics of Fluids*, 9(3):766–775, 1997.

[4] Zimon, V., Barbato, M. Modellizzazione e Teorizzazione per Combustione Premiscelata e Parzialmente Premiscelata. Internal report, CRS4 Research Centre,- CRS4-Tech-Rep, October 1999.

[5] Turns Stephen R. An introduction to combustion. In *Concepts and applications*. McGraw-Hill, 1996.

[6] Andrews, G. E., and Bradley, D. The Burning Velocity of Methane-Air Mixtures. *Combustion and Flame*, 19:275–288, 1972.

[7] Metghalchi, M.., and Keck, J. C. Burning Velocity of Mixtures of Air with Methanol, Isoctane and Indolene at High Pressures and Temperatures. *Combustion and Flame*, 48:191–210, 1982.

[8] Barnett H. C. and Hibbard R. R. "Basic Considerations in the Combustion of Hydrocarbon Fuels with Air". Technical Report 1300, NACA, 1959.

[9] Law, C.L., and Egolfopoulos F.N. A Unified Chain-Thermal Theory of Fundamental Flammability Limits. In *Twenty-Fourth Symposium (Int.) on Combustion*, page 137. The Combustion Institute, 1992.

[10] Moreau, P.,. Turbulent Flame Development in a High Velocity Premixed Flow. *AIAA Paper 77-49, AIAA 18th Aerospace Science Meeting*, Jan. 24-25 1977, Los Angeles, CA.

[11] Mulas, M., Stalio, E. and Talice M. Development and Implementation of Turbulence Models in the Combustion Code Ares. Internal report, CRS4 Research Centre,- CRS4-Tech-Rep, 2001.

[12] Boris Jay P. Oran Elaine S. In Seebass R., editor, *Numerical Approaches to Combustion Modeling*, volume 135 of *Progress in Astronautics and Aeronautics*. American Institute of Aeronautics and Astronautics, 1991.

[13] Libby, P.A. and Williams, F.A. editors. *Turbulent Reacting Flows*. Academic Press, 1994.

[14] Borghi, R. and Destriau M. *La Combustion et Les Flammes*. Éditions Technip, 1995.