Methane Combustion and Heat Transfer in a Turbo-gas Combustor using a Net of Ideal Reactors

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1. Introduction

The simulation of the heat exchange of process reactive in three-dimensional turbulent flows is a difficult subject on account of the strong interaction among fluid dynamic and kinetic. Even if it is possible draw the equations that regulate the process, the resolution of these equations requires enormous time of calculation and, however, the result is tie to the model of the turbulence used. A possible approaches consists in simplify the problem, privileging the kinetic aspect in comparison with that fluid dynamic or viceversa.

In this work an intermediary approach is proposed. A series of ideal reactors is used for the combustion of the mass of the single zones in with the combustor can by divided. What characterises the combustion of the single zone is the air-fuel ratio, determinate from the fluid dynamics. Such air-fuel ratio is able be statistically drawn by a function that holds in count, with opportune parameters, of the " quality " of the mixture.

2. Methodology

In the diffusive combustors, the fluid dynamics influences strongly the mixture among fuel and air, determining, in the primary zone, the distributions of the equivalence ratio. In the secondary instead, the distribution of the hole of dilution and the entry speed of the air determine the residence time and the cooling of the burnt gas coming from the primary zone, with consequent influence on the low temperature dissociation and re-association reaction. In principle, the field of motion in a reactive environment it may lead to two extreme situations in the fluid volume: absence of axial mixing or a complete axial mixing. The first situation is model with a plug flow Reactor (PFR), while the second case is model with a continuous stirred tank Reactor (CSTR). Among this two extremes, a statistic function it may furnish the mixture "degree of mixing" (air-fuel equivalence ratio) in every section of the combustor and then it may create a net of ideal reactors (PFR and CSTR) that introduces the same distribution curve of the permanence time of the system that is wants study.

The Beta statistical distribution to four parameters is presumably the function that better brings near to the dynamics of the mixture. Such function can be express as[1]:

$$f_B\{\phi,\phi_{\min},\phi_{\max},\lambda_1,\lambda_2\}=\frac{\Gamma(\lambda_1+\lambda_2)}{\Gamma(\lambda_1)\Gamma(\lambda_2)}\left(\frac{\phi-\phi_{\min}}{\phi_{\max}-\phi_{\min}}\right)^{\lambda_1-1}\left(1-\frac{\phi-\phi_{\min}}{\phi_{\max}-\phi_{\min}}\right)^{\lambda_2-1}\frac{1}{\phi_{\max}-\phi_{\min}} \qquad (1)$$

where ϕ is the independent variable (air-fuel equivalence ratio), ϕ_{min} and ϕ_{max} represents the limit of the field of variation ϕ, λ_1 and λ_2 the form parameters whose variation consents to get the different configuration and Γ the Gamma function .

Forming the hypothesis that all the configurations have the same mode, it is possible to impose a relationship of dependence among the two parameters form as

$$\lambda_{1=}\frac{\phi_{\max}+\phi_{\min}-2\phi_{\mathrm{m}}}{\phi_{\max}-\phi_{\mathrm{m}}}+\frac{\phi_{\mathrm{m}}-\phi_{\min}}{\phi_{\max}-\phi_{\mathrm{m}}}\lambda_2$$

The simple variation of λ_2 allows one to get any distribution of the air-fuel ratio into the combustion. It may think so that λ_2 represents the mixing goodness index: much more elevated will be this value, many better will be the combustion.

Hypothesising to divide the primary zone of the combustor in a certain section number, the dynamics of the combustion along it may be described, in sufficiently appropriate way, assuming a linear relationship among the form parameter λ_2 and the current section N_S:

$$\lambda_2 = aN_s + b$$

where the constant a influences the speed with which evolves the combustion and the b parameter defines the situation of departure. In after all the probability density function is able to be express simply in term of ϕ and Ns:

$$PDF(\phi,N_s)=\left\{B^{-1}[\lambda_1(N_s),\lambda_2(N_s)]\right\}\left(\frac{\phi-\phi_{\min}}{\phi_{\max}-\phi_{\min}}\right)^{\lambda_1(N_S)-1}\left(1-\frac{\phi-\phi_{\min}}{\phi_{\max}-\phi_{\min}}\right)^{\lambda_2(N_S)-1}\frac{1}{\phi_{\max}-\phi_{\min}} \qquad (2)$$

In this work the combustor is divided in ten sections in the primary zone and six sections in the secondary zone. The Fig. 1 shows the variation of the PDF in the ten section of the primary zone, for a typical value of the parameters a and b.

The Fig.s 2 and 3 show the complete computational scheme of the combustion. The figures bring symbolically the reactor net and the currents. The air in the primary zone comes divided up into ten section of the combustor proportionally to the hole of entry. To every section competes a value of ϕ coming from equation (2), a time that the parameters a and b are fixed base on the particular type combustor and obtainable of given experimental. Every section is then divided in ten equilibrium stadiums. In this part of the combustor the reactions are in equilibrium condition because the level of temperature is high. To the exit of the primary they will have then the composition, the temperature and the flow of all the components of the products of combustion. Such system comes then connected with the secondary where the combustion has a kinetic scheme described later on. In this case operates with a PFR reactor.

In order to study a configuration of ideal elements in serious-parallel, a computer code had developed that allows to analyse system even much complex, as long as destitute of recycle. The code requires the knowledge of the graph of the net that is intended study. The knots of the graph are the ideal apparatuses, while the connections among the knots represent the currents. The unknowns of the problem are the composition, the temperature and the flow of some intermediary and the exit currents.

The Methan kinetic scheme used to the simulations includes 43 chemical species and 182 reactions. The kinetic constants are treated for the greatest part from Basevich[2]. For some reactions, the most important, are used the given kinetic of the database of the National Institute of Standards and Technology (NIST[3]). The kinetic scheme contains even a series of formation and consumption reaction of nitrogenous composes [4,5]. Such compounds play a fundamental role in the study of environmental implications of the combustion with air, being they among the principal causes of the air pollution. The determination of the production of this pollutants at the exit of the apparatuses of combustion are then one of the more important information's furnished from the use of detailed kinetic models.

3. Analysis of the result and conclusions

The previous methodology has been applied to a series of different combusts to verify the applicability. The Fig. 4 shows the progression of the temperature along a plan for two of the ten section of the primary. The values are reported in term of mass fraction with the temperature in a class (in %). How to is seen, the comparison is acceptable, expecially for the distribution 2 and 3. The Fig. 5 reports instead the change of three burnt species long the axis of a combustor working with a β of about 30 and a τ of about 5 (aeronautical combustor type). The dots in the figures at the end of the combustor displays the mean value of the concentration of the species as result from [6]. How to is seen, the different distributions influence the estimation above all of the values of the No_x. All that is congruence with the physical aspect: combustions with distributions " improves " (with more rapid mixtures and homogeneous about to the mean value as the distribution 5) bring to the reduction of the quantity of CO issued but, on account of the combustion temperature more elevated, of a greater emission of No_x.

The here proposed methodology is promising for predictions of the heat exchange and emissions of a turbo-gas combustor, without a punctual calculation of the fluid dynamics: the beta function to four parameters allows, with a wide flexibility, to describe rapidly the connection among fluid dynamic and the combustion. Of against, the kinetic model appear sufficiently detailed to catch the effects of the various components of the combustor on the emissions.

The limit of the method is sufficiently clear: any type of " phenomenological " (or zero-dimensional) model as the present is not a design tool but an analysis tool, more sophisticated than the simple kinetic model, a time that it is calibrated to a particular combustor.

4. Bibliography

1. Bury K. V., 1975, "Statistical Models in Applied Science" John Wiley Sons, Inc. U.S.A.
2. Basevich V. Y. A., 1987, "Chemical Chinetics in the Combustion Processys: A Detailed Chinetic Mechanism and its Implementation", Prog. Energy Comb. Sci, vol. 13, pp 199-248.
3. Mellard V. G., Westley F., Herron J.T., and Hampson R.F., 1992, NIST Chemical Chinetics database Ver 4.0, NIST Standard Reference Data, Gaithersburg (MD).
4. J. A. Miller, and C.T. Bowman, "Mechanism and Modeling of Nitrogen Chemestry in Combustion", Prog. Energy Comb. Sci, vol. 15, pp 287, 1989.
5. Fenimore C. P., 1970, "Formation of Nitric oxide in premixed hydrocarbon Flame", 13° Symposium (Int) on Combustion, The Combustion Institute, pg 373.
6. A.F. Bicen, D. Tse, J.H. Whitelaw, "Flow and Combustion Characteristics of an Anular Combustor", Combustion and Flame 72, 1988, pp 175-192.
7. M.V. Heitor and J.H. Whitelaw, Combustion and Flame 64, 1986, pp. 1-32
8. W.P. Jones, H. Toral, Combustion Science and Technology 31, 1983, pp. 249-275.

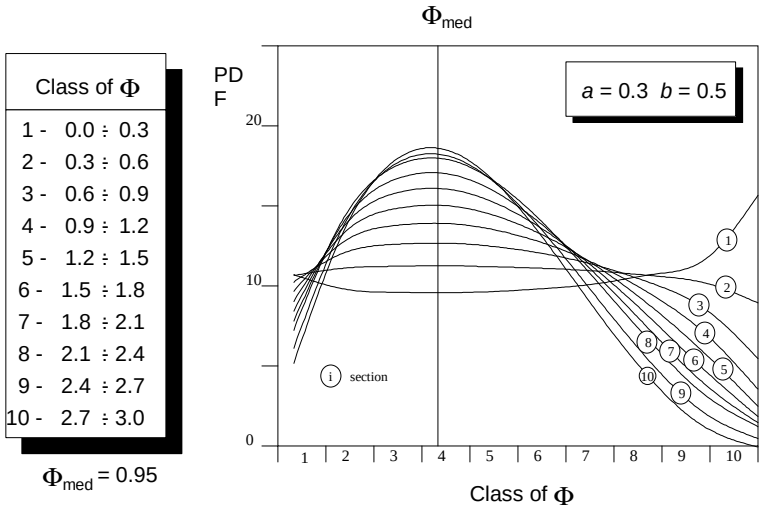

Fig. 1- *probability density function of the mass in the 10 section of the primary for 10 equivalence class, for typical values of* ***a*** *and equation* ***b*** ***of equation (2).***

Fig. 2 – *Compatation scheme of the primary zone*

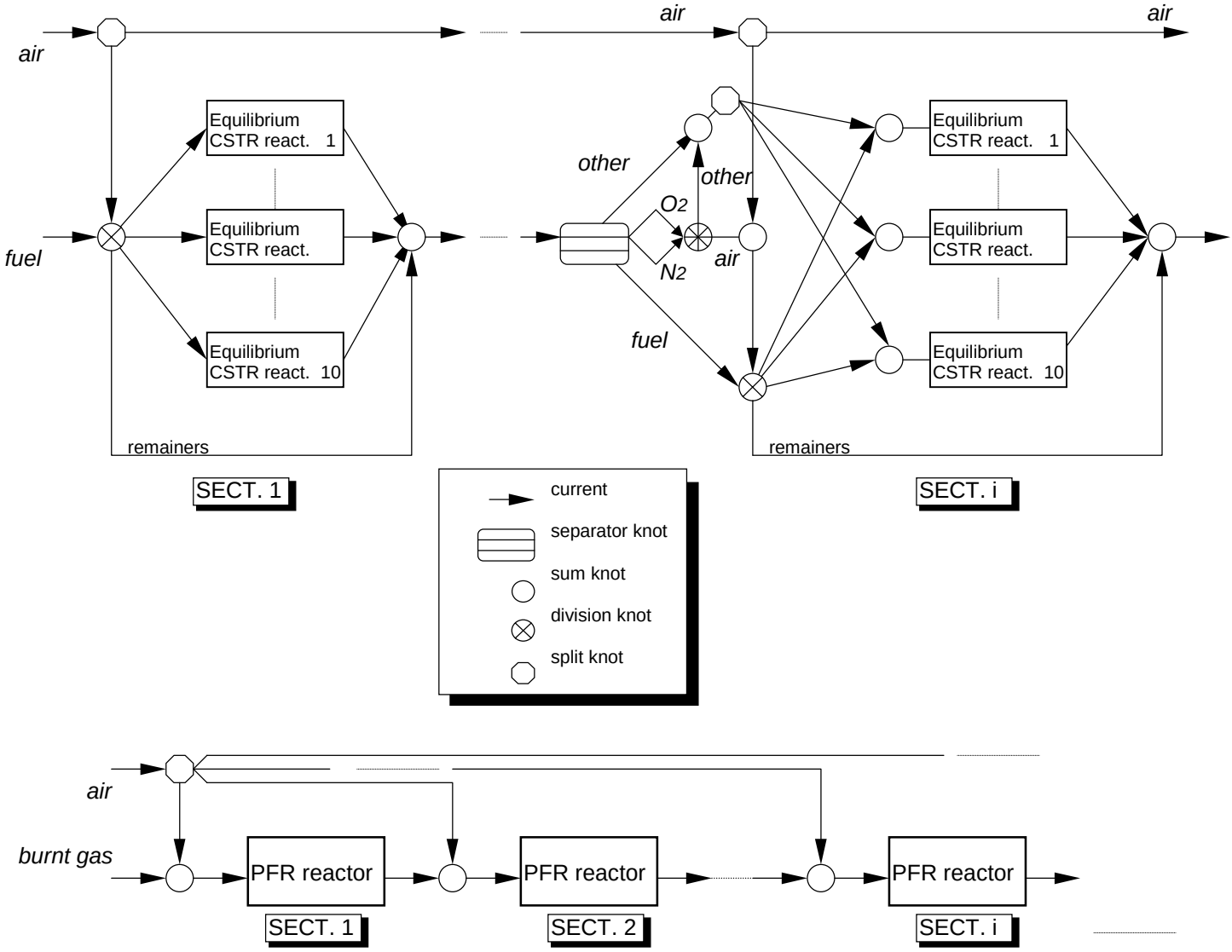

Fig. 3 – *Compatation scheme of the dilution zone*

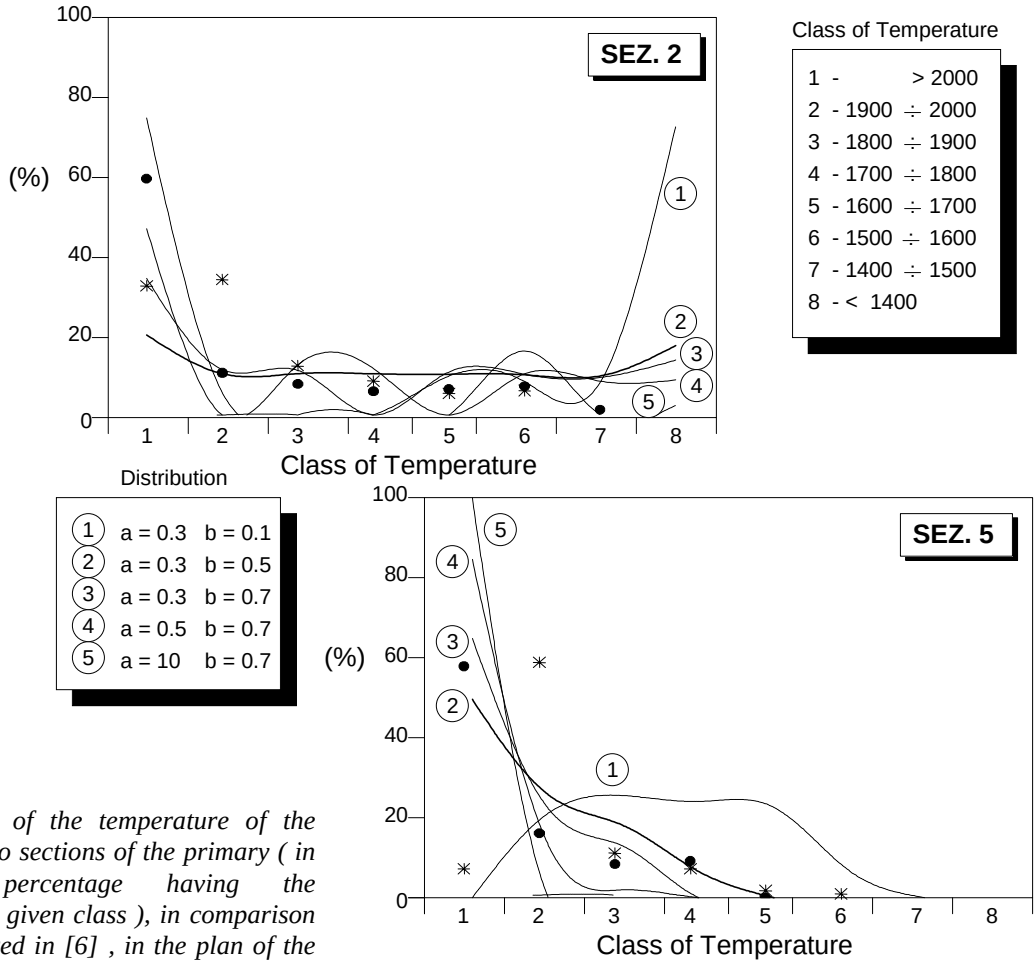

Fig. 4-*variation of the temperature of the burnt mass in two sections of the primary (in term of mass percentage having the temperature in a given class), in comparison with that measured in [6] , in the plan of the jet (●) and in an orthogonal one (✳).*

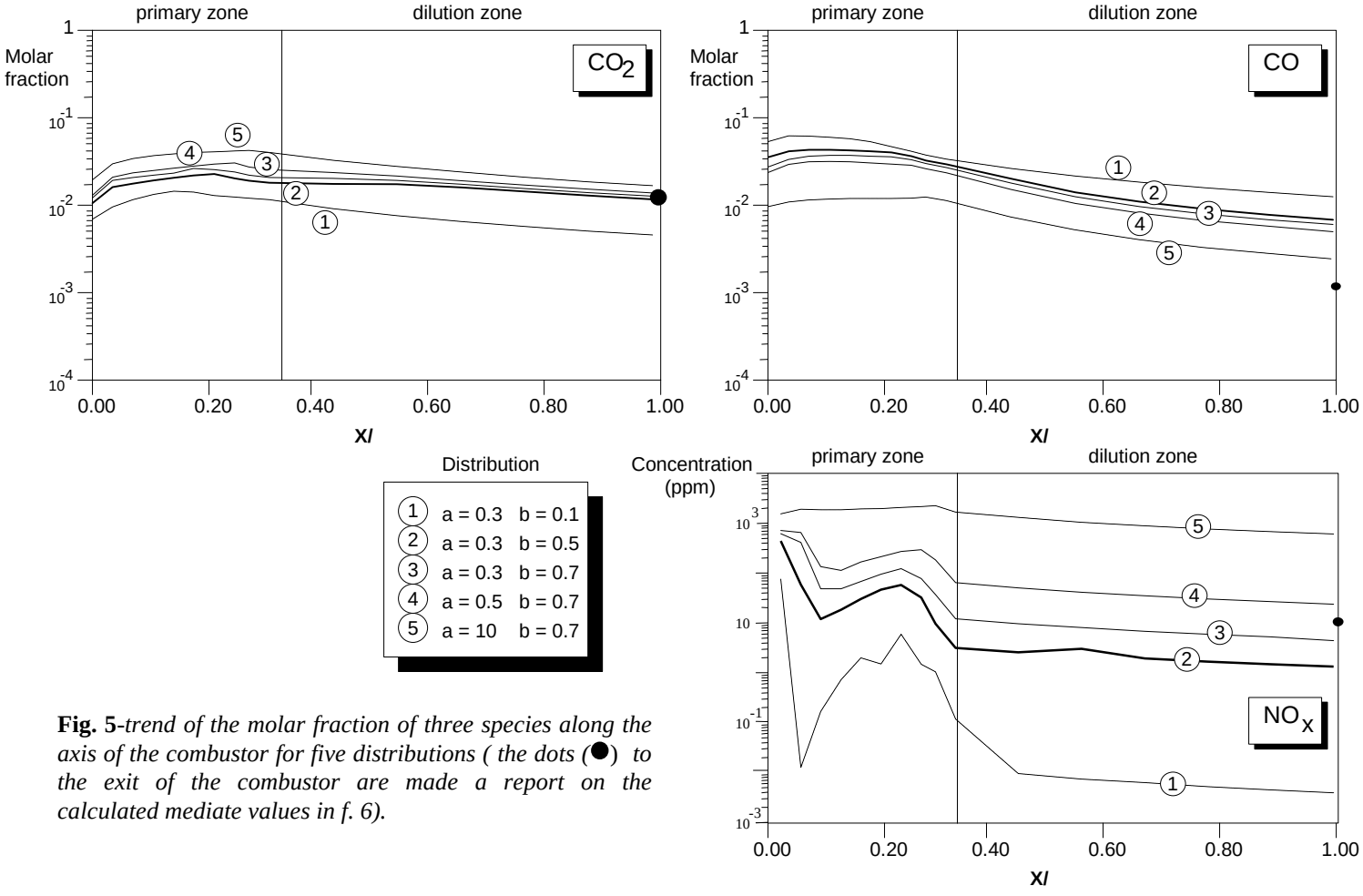

Fig. 5-*trend of the molar fraction of three species along the axis of the combustor for five distributions (the dots (●) to the exit of the combustor are made a report on the calculated mediate values in f. 6).*