Detailed Chemistry Prediction of Time-Dependent Turbulent-Combustion within a Gasoil-Fueled Rapid-Mix Burner-Combustor System

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ABSTRACT

The paper, in its first part, reports synthetically about the latest conceptual and numerical developments implemented into the CRFD (Computational Reactive Fluid Dynamics) parallel/clusterized solver NastComb, discussing in particular its most recently programmed detailed-chemistry mechanism. This scheme adopts a PASR (Partially Stirred Reactor) approach together with an SGI (Sub Grid Interaction) model in order to represent the turbulence-chemistry cross-influences. In the second part, preliminary results are given and discussed of the application of the code to an experimental, gasoil-fueled, LRPM (Liquid-fuel Rapid Pre-Mix) gas-turbine burner, characterized by ultra-low emissions. Comparisons with measured temperature data turn out quite positive, whilst the detailed chemistry provision allows to go deep into the mechanisms of radical and pollutant species formation.

INTRODUCTION

The so-called LRPM (Liquid-fuel Rapid Pre-Mix) gas-turbine burner technology, under development at DIMSET/SCL, Savona Combustion Laboratory, since 1997, is a liquid-fuel rapid-mix technique which, for ultra-lean equivalence ratios, has recently attained, with gasoil fuel, the ultra-low emissions target, in terms of NOx and CO levels well constrained within the "one-digit ppmv" range, at atmospheric pressure and 15% O_2. This type of performance is achieved, together with excellent stability of the flame process, by taking advantage of the localized injection of the liquid fuel directly into the flow-field locations where, by design, the turbulence kinetic energy, or, more specifically, its dissipation rate, attains its peaks, thus dramatically improving the fuel droplets' disaggregation, pre-vaporization and rapid mixing with air [1,2].

In order to support theoretically the development of the LRPM burner design, as well as to help interpret the parallel experimental investigations, with particular attention addressed to the crucial two-phase liquid-fuel rapid-mixing process in presence of the counter-flow influences coming from the flame process, extensive parametric applications of fully 3D time-dependent numerical predictions have been performed in the years. The turbulent reactive Navier-Stokes analyses have been pursued by applying, with parametric modalities, NastComb, the time-dependent CRFD (computational reactive fluid dynamics) Navier-Stokes solver developed at DIMSET during many years [2,3,4,5] by progressively converting to gas-turbine applications and extending its forefather, namely KIVA-3V code. To be noticed, without the detailed, extensive support of these numerical analyses, hardly the final, optimised burner configuration would have been achieved.

MOST RECENT EXTENSIONS TO SOLVER NASTCOMB

The governing equations for 3D, fully time-dependent, turbulent, variable-density, reactive flow, in presence of conduction and radiation, formerly of favre-averaged formulation, have

recently been further extended toward an ensemble-favre-averaged scheme, in order to take full advantage of the Markovian revisitation performed on its turbulence model:

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = -\nabla \cdot <\rho' \mathbf{u}'>$$

$$\frac{\partial}{\partial t} \overline{\rho} U_i + \frac{\partial}{\partial x_j} \overline{\rho} U_i U_j = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(-\overline{\rho} <u_i' u_j'> -U_j <\rho' u_i'> -U_i <\rho' u_j'> \right) + \frac{\partial}{\partial x_j} \overline{\mu} S_{ij}$$

$$\frac{\partial}{\partial t} \overline{\rho} E + \nabla \cdot (\overline{\rho} \mathbf{U} E) = \nabla \cdot \left(-\overline{\rho} \langle e' \mathbf{u}' \rangle - E <\rho' \mathbf{u}'> \right) - (P \nabla \cdot \mathbf{U} + <p' \nabla \cdot \mathbf{u}'>) +$$

$$+ \nabla \cdot (\overline{\kappa} \nabla T) + \overline{\mu} S_{ij} \frac{\partial U_i}{\partial x_j} + Q_{rad} + Q_{chem}$$

The above mentioned turbulence model, developed and validated along several years, is a three-equation, non-linear eddy-viscosity approach based on the so-called "Two-Scale Direct-Interaction Approximation" (TSDIA) with a Markovian simplification (MTS) for the solution of the approximate equations for fluctuations [6,7]. The model accounts for variable-density effects via a transport equation for the density-variance, which corrects the eddy-viscosity, and is thus particularly suited to track the interactions between turbulence and the density variations as induced by the reactive field.

For liquid fuels, the treatment of fuel spray dynamics in NastComb was originally based on the KIVA-related TAB model (Taylor Analogy Break-up), typically showing the known inconsistency of progressively segregating the droplets' populations into two separate, far-apart families, one with only the very large and the other with the very small droplets. In order to reach a better agreement with experimental available results for gas turbine injectors, in the numerical jet description a distinction has been introduced between the jet blobs' and the droplets' breakup models. The breakup is now supposed to be due to the growing of some instability waves on the liquid surface until they reach dimensions similar to those of the liquid blob. The primary break-up of the jet column is then related to the Kelvin-Helmholtz (KH) instability induced by the relative velocity at the interface. Among the many wavelengths, the one which grows faster is considered responsible for the break up (i.e. the most unstable one). While the blobs primary break up is mainly influenced by the Kelvin-Helmholtz waves' grow-up process, the secondary break up of the droplets, formed from the blobs, is now modeled considering also other types of instabilities, such as the so called Rayleigh-Taylor (RT) instability, related to the acceleration experimented by the liquid drops. In the same way as before, expressions for the fastest-growing wave characteristics are derived, as well as for the relative breakup time [2,8,9]. The introduction of this new breakup model in NastComb code has greatly enhanced its flexibility and accuracy: indeed, the different break-up models, to be used in competition among themselves (in terms of time to reach break-up), can better capture the many different physical aspects involved in the problem of correctly predicting the fuel spray evolution, so crucial for performing reliable analyses of quasi-premixed combustion.

In Nastcomb solver a detailed, non-equilibrium, continuous-field, time-dependent 3D radiation model has been introduced, and made interactive with the overall turbulent reactive thermo-fluid-dynamical solution. Originally the model, of a "neutronic" character, was developed within a 2D, equilibrium assumption for the radiation diffusion treatment. Then, the scheme has been extended to nonequilibrium diffusion, wherein the gas and the radiation fields can have different temperatures, and flux-limiters are adopted to extend the diffusion theory to optically-thin regions, with also 3D capability [4]. In synthesis, the transport

equation for the radiation energy-density is solved fully coupled with the gas energy-density equation. The coupling terms which relate the radiation energy density to the fluid energy density are large when the photon mean-free paths due to molecular collisions are small ("optically-thick" regions) whilst the opposite is true in "optically thin" regions.

As a rule, in the previous versions of solver NastComb, combustion simulation was performed by developing and implementing, along the years, several formulations of quasi-global, partial-oxidation, schemes, adjoined with limited sets of elementary reactions (12 to 16 species, 26 to 34 reactions) with the aim of improving the chemistry representation. In order to take care of turbulence effects, the expression of the total combustion time τ_c was evaluated as the sum of a molecular time-scale τ_l , taken as the inverse of the quasi-global reaction rate, and a turbulent time-scale τ_t , related to the eddy turnover time [10].

An extremely recent, detailed chemistry, parallel/clusterised version of NastComb has been set-up and made operative on a set of 6 two-processor pc's. This scheme, taken from [11,12], is based on the PASR, "partially stirred reactor", concept, by which a computational cell volume is assumed as split in reactive and non-reactive regions. Due to this volume sub-partition, the chemistry-turbulence interaction is allowed to produce favorable conditions for combustion in certain parts. Within a volume fraction K^*, the mixture initial concentration c^0 undergoes a reacting process to concentration c, then mixes with the unreacted mass of the reactor forming the cell output concentration c^1, all this during one time step τ, which thus assumes the meaning of the local residence time. With interpolation we get:

$$c^1 = \kappa^* c + (1 - \kappa^*) c^0 \tag{1}$$

The reactor concentration c is information on a sub-grid scale. In order to express it in terms of grid resolved quantities, let's assume that the time, for the initial concentration c^0 to reach the final concentration c^1 , be equal to the integration time step τ . The time for mixing c with c^0 to get c^1 is, thus, the mixing or micro-mixing time τ_{mix}. Assuming the rates of these two mechanisms are equal, it is possible to evaluate the chemical source terms $f(c)$ and also to identify the reactive volume fraction K^* as given in the expressions:

$$f(c) = \frac{c^1 - c^0}{\tau} = \frac{c - c^1}{\tau_{mix}} \qquad\qquad \kappa^* = \frac{\tau}{\tau + \tau_{mix}}$$

At this point, always following [11,12], in order to solve the problem of the still unknown concentration c in eq.(1), the "reference species" technique is introduced, as an estimate of the shortest chemical time scale τ_{chem} : indeed, strong time dependence (stiffness) of the chemical source term directly affects the choice of the relevant time integration step τ. The reference species is defined as the species closest to being driven to zero-concentration limits, and it can be shown to correspond to the reaction partner of the species with the largest concentration. Calling with c_{max} this latter concentration, which is partner to the former (i.e. c_{ref}) in the reaction, the relevant chemical time-scale can be evaluated as:

$$\tau_{chem} = \frac{1}{k_f \cdot c_{max}}$$

where k_f is the forward rate coefficient of the reaction. It is now possible using eq. (1) for exclusion of the sub-grid concentration c , to write the chemical production term $f(c)$ in terms of grid-resolvable information only:

$$f(c) = f(c^1) - \frac{c^1 - c^0}{\tau} \frac{\tau_{mix}}{\tau_{chem}} = \frac{c^1 - c^0}{\tau} \tag{2}$$

which can be finally rearranged, after redefinition of a new volume fraction K, as:

$$f(c) = \kappa \cdot f(c^1) \qquad\qquad \kappa = \frac{\tau_{chem}}{\tau_{chem} + \tau_{mix}}$$

The above *f(c)* is the representation of the chemical source term of mass balance equation which, modeled on the basis of grid-resolved information only, can be directly evaluated by solver NastComb by using the reaction rate in Arrhenius formulation.

In order now to properly account for the turbulence-chemistry interaction process, a correct definition of the micro-mixing time τ_{mix} is important. The micro-mixing time-scale can range from the break-up time-scale of large eddies down to the Kolmogorov time-scale of the smallest eddies. A subgrid micro-mixing time in relation to the RNG subgrid viscosity could be used [11], whilst in [12] the classical Kolmogorov expression is used for the micro-mixing time with the molecular viscosity replaced by the effective viscosity.

However, taking advantage of the markovian revisitation of NastComb's TSDIA turbulence model, the mixing time-scale can be directly taken from the markovian formulation of the sub-grid eddy viscosity expression [6,7]. Actually, in NastComb, this expression is even successive to the evaluation of its characteristic time-scale, this latter thus being determined at a more fundamental level than the former.

APPLICATIONS TO GASOIL-FUELED LRPM BURNER

As above said, there are presently two versions of solver NastComb, with different reactive mechanisms, one based on quasi-global, partial oxidation schemes adjoined with limited sets of elementary reactions, the other one implementing the above mentioned detailed chemistry scheme under the PASR approach, with its SGI "sub-grid interaction" model. Both versions have undergone complete parallelization and are now executable on a cluster of 6 two-processor pc's in shared-memory mode. They have been applied, both for technological design as well as for experimental validation purposes to the liquid-fuel rapid-mix burner, named LRPM, installed on a dedicated, atmospheric pressure, air-preheated, test-rig available at DIMSET-SCL (Savona Combustion Laboratory) [13]. The burner, fueled with gasoil, has already attained the target of ultra-low emissions jointly with a remarkably stable regime, for ultra-lean equivalence ratios and air preheating levels of about 330 °C.

As far as temperature distributions are concerned, numerical predictions, obtained with a quasi-global mechanism, already turned out in good agreement with experimental data [2].

The very recent, so far unpublished and anyhow preliminary, numerical predictions here presented are referred to the detailed-chemistry version of NastComb. In order to characterize the most important properties of gasoil fuel, together with its combustion products and emissions including particulate inception, a detailed chemistry mechanism has been implemented, in Chemkin format, involving 232 species and about 1500 reactions, suitable to model combustion and pyrolisis of species up to n-dodecane [14,15].

In Fig.1 the internal view of the eight-vane radial-inflow "stabilizer" is given: in order to enhance its rapid-mix capability, the liquid fuel is injected radially inward, directly near the inlet of each one of its 8 vane passages. Fig.2 shows the fuel droplets' behaviour as predicted, in "competitive" mode, by NastComb's different spray modelisations. Interestingly, the "tail" of the droplets' cloud, after getting thicker near the axis of the discharge "eye" of the swirler, appears as undergoing rapid evaporation and mixing ahead of entering the combustor proper. Fig.3 presents the experimental temperature distributions in three successive axial stations within the cylindrical combustor, compared with NastComb's predictions: cross-comparisons turn out quite positive, almost everywhere. Notice the absence of peak temperatures above 1350 °C and a very smooth temperature distribution in the whole chamber, confirming attainment of adequate premixing levels ahead of the flame front. The complete numerical

prediction of the temperature distribution within the meridian plane of the overall LRPM system is shown in Fig.4 .
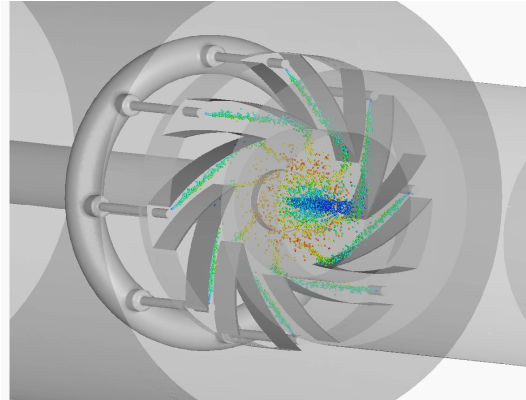

Fig.1 - LRPM radial-inflow swirler

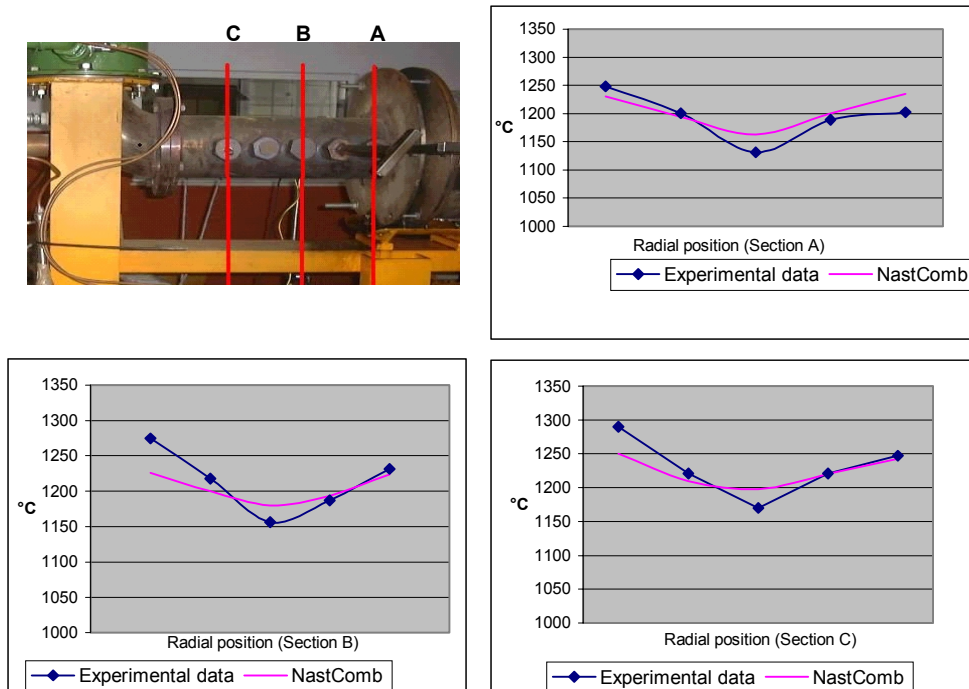*Fig. 2 - Spray dynamics prediction within the rapid-mix swirler passages (code NastComb)*

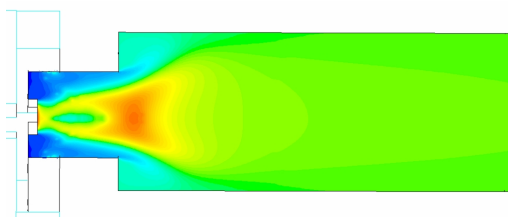*Fig.3 - Experimental and numerical temperature distributions*

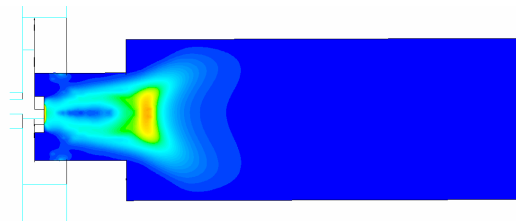*Fig. 4 – Temperature prediction (min: 585 K – max 1779 K)*

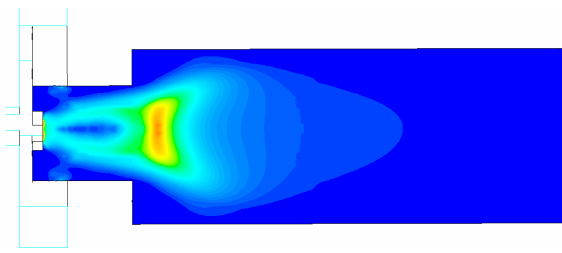*Fig. 5 – Formation of OH (mole fraction max = 1.27 10^{-4})*

Fig. 6 – Formation of OH$_2$
(mole fraction max : 5.37 10^{-5})

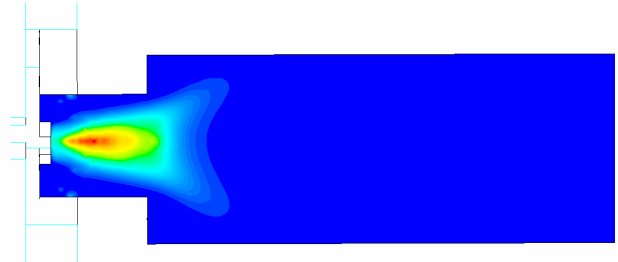*Fig. 7 - Formation of C$_2$H$_2$*
(mole fraction max: 1.44 10^{-6})

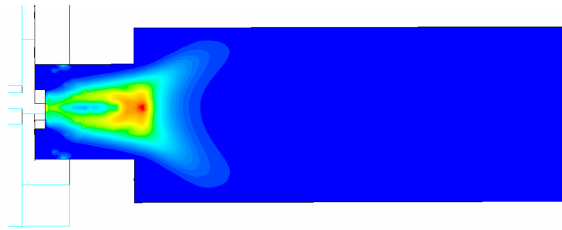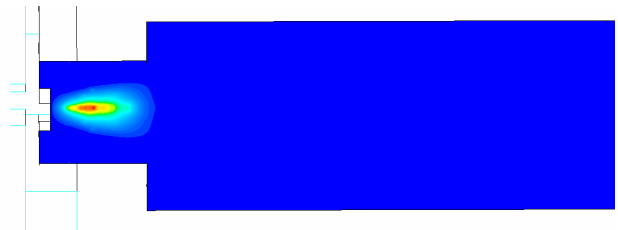*Fig. 8 – Formation of CH$_{2s}$*
(mole fraction max : 7.01 10^{-5})

Fig. 9 - Formation of C$_s$
(mole fraction max: 1.20 10^{-6})

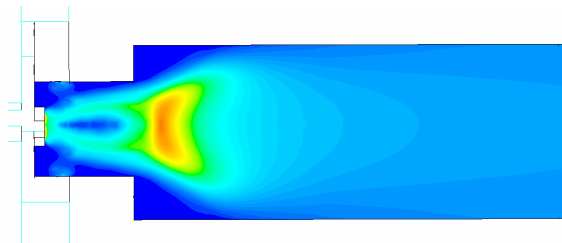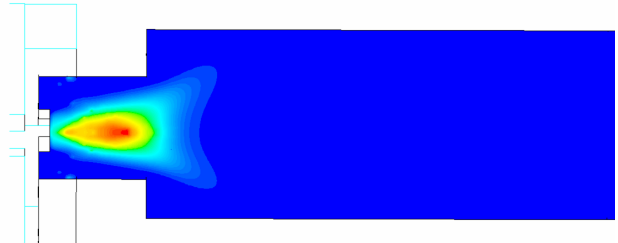*Fig. 10 – Formation of NO*
(mole fraction max : 5.97 10^{-4})

Fig. 11 - Formation of CO
(mole fraction max: 2.45 10^{-2})

Figs.5 through 11 show the formation of some relevant radical species as well as pollutants, mostly in dependence of local temperature behavior. Interestingly, O-H chemistry appears as very much "tuned" with the highest temperature levels (e.g. OH and OH$_2$ formation in Figs.5 and 6, respectively) attained well inside the combustor. On the other hand, C-H chemistry related to pollutant precursors such as CH$_2$ singlet (in Fig.8, linked to prompt NOx formation) and notably acetylene (in Fig.7, related to particulate inception through the well assessed kinetics of aromatics) appears as taking place well ahead of the flame front, namely where increasing levels of temperature, but anyhow far from its peaks, interact with the evaporating droplets' cloud, typically in the still high droplets-density region near the discharge of the swirler (see Fig.2 and 9). This turns out clearly confirmed also by the location of the "graphitization" process as depicted in Fig.9.

Furthermore, it can be observed that the locations where O-H chemistry is most active correspond to the peak formation of NO (thermal and prompt, in Fig.10), whereas the locations characterized by the above discussed C-H chemistry appear as mostly tuned to peak CO-formation. Notice that no downstream, equilibrium-related, CO formation shows up, due to the ultra-lean equivalence ratio (around 0.39) and, possibly, to an adequate premixing-level attained ahead of the flame front.

CONCLUSIONS

Though preliminary, the first results obtained by applying the detailed-chemistry version of solver NastComb to the LRPM burner-combustor system appear important toward further assessment of its optimised-design parameters and deeper interpretation of the processes

related to its thermo-chemical performance and emissions. To be noticed, the positive cross-comparisons between theoretical predictions of temperature distributions and experimental data succeed in validating the overall analytical and numerical structure of NastComb with all its submodels, inclusive of the crucial spray dynamics modelisations. The detailed chemistry mechanism, jointly with the turbulent-chemistry interaction model above discussed, appear as powerful tools in order to investigate deeply the processes usually ill-predicted by current-generation computer codes, namely pollutant emissions and ignition delay.

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