Numerical Simulation of 3D Reacting Flow in Gas Turbine Combustors. Part I: The NastComb Solver.

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ABSTRACT: The paper is splitted in two parts. In the present one, a description will be given of the theoretical and numerical aspects of the turbulent reacting flow solver NastComb, developed at DIMSET since the early 1990s. In particular, attention will be focused on the recent implementations of a 3-equation turbulence model for compressible flows, of an extended combustive model and of an accurate solution strategy accounting for radiation effects. These features, along with the use of suitable mesh configurations, have further enhanced the overall predictive capability of the code to highly competitive levels even in presence of complex simulation tasks.

INTRODUCTION

Over the last years, CFD (computational fluid dynamics) has attained significant advancements in accurately predicting turbulent flows by means of improved modeling capabilities and higher order numerical techniques. The parallel speed up in CPU frequency rates and the development of clustering tools, by which portions of the same numerical problem can be assigned to several inter-linked processors, greatly enhance convergence times for complex simulations. On the other side, in presence of reacting flows, design and parametric optimizations of combustion systems components (injectors, burners, liners, combustors, etc.) pose highly difficult challenges, and still have to rely on extensive, and expensive, performance testing. The problem, for this latter strategy, is that in presence of high temperatures, pressures and flow rates in the combustor, the situation is far from affording comprehensive experimental data to be taken easily, or to be taken at all. In this context, CFD is recently attaining a peculiar and important role, namely that of taking strategic advantage from experimentation in order to complementing it, and thus becoming a more reliable development tool for the gas turbine designer: with the help of well focused experimental data, to be utilized also for validation purposes, numerical

simulations can efficiently track the reacting-flow processes (physical and chemical) inside the combustor and assess the performance feedback of the system to changes in design parameters or in geometrical features. All the above can be considered as the motivating, conceptual "scenario" of the numerical research here presented.

The paper is splitted into two parts. This Part I presents structure and main characteristics of a recent, combustion-specialized, extension (named NastComb) of code Nast[1], a previously fluid-dynamical-only Navier-Stokes solver. This fully time-dependent, 3D, numerical tool is based, for each time-step advancement, on a lagrangian scheme, followed by a grid-restoring eulerian phase. The turbulence model specifically developed and applied is rather peculiar, involving a 3-equation scheme capable of accounting for anisotropy and compressibility effects. Combustion modeling relies on a partial-equilibrium approach based on a quasi-global scheme, extended with a proper set of elementary reactions. Turbulence and chemical kinetics interactions are taken into account through turbulence-dependent corrections operated onto the Arrhenius rates. Radiation effects are also accounted for by a radiation-energy transport equation which is solved fully coupled with the gas internal energy equation.

Part II of the paper (same Ref.) is application-oriented, dealing with the numerical study of an industrial gas turbine combustor, the Ansaldo-Siemens V64.3A (annular) model. Detailed 3D maps of velocities, temperatures, specific densities and turbulence quantities at steady-state are given and discussed, together with a very first (tentative) prediction of possible unstable responses of the combustive system to pressure perturbations. A few experimental data are utilized for validation, exactly in the spirit of above said "complementing" of theoretical data with experimental evidence.

THE COMPUTATIONAL MODEL

NastComb[2] is the combustive extension of Nast, a finite-volume, 3D, fully time-dependent, compressible thermo-fluid-dynamical Navier-Stokes solver of ALE (arbitrary lagrangian-eulerian) family[3], in which every time-step consists of a lagrangian phase, with the flow velocities applied to the (moving) grid vertexes, followed by a convective phase, i.e. a rezoning of the (updated) flow field, performed by displacing the grid back to its initial position. A monotone, nearly second-order, (QSOU) differencing scheme[3] is applied for convection, with use of cell-face velocities in order to lower numerical diffusion. To increase numerical efficiency, a pressure-gradient scaling (PGS) algorithm[3] is activated whenever flow velocities are particularly low. Grid types are staggered, boundary fitted, structured, with hexahedral cells. The governing equations for turbulent reactive flow, strictly speaking in favre averaged terms, but re-interpreted as ensemble-averaged for the turbulence-related terms[5], can be written as follows:

$$\frac{\partial(\overline{\rho}\{Y_m\})}{\partial t} + \nabla \cdot (\overline{\rho}\{Y_m\}\mathbf{U}) = \nabla \cdot \left[\overline{\rho D}\nabla\{Y_m\}\right] + \{\omega_m\} \qquad (1)$$

$$\frac{\partial}{\partial t}\overline{\rho}U_i+\frac{\partial}{\partial x_j}\overline{\rho}U_iU_j=-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_j}\left(-\overline{\rho}\{u_i'u_j'\}\right)+\frac{\partial}{\partial x_j}\overline{\mu}S_{ij} \tag{2}$$

$$\begin{aligned}\frac{\partial}{\partial t}\overline{\rho}E+\nabla\cdot\left(\overline{\rho}\mathbf{U}E\right)&=\nabla\cdot\left(-\overline{\rho}\{e'\mathbf{u}'\}\right)+\\&-P\nabla\cdot\mathbf{U}+\nabla\cdot\left(\overline{\kappa}\nabla T\right)+\overline{\mu}S_{ij}\frac{\partial U_i}{\partial x_j}+Q_{ch}+Q_{rad}\end{aligned} \tag{3}$$

where Y_m is the mass fraction of species m and ω_m is its chemical source term; D is Fick's (single) diffusion coefficient; S_{ij} is the mean strain tensor; E is the mean internal energy; Q_{ch} is mean source term for chemical heat release, whilst Q_{rad} is mean exchange term for radiation heat.

Very recently, a compressible-turbulence (and variable-density) model, called "Two Scale Direct Interaction Approximation" with Markovianized simplification (TSDIA/ MTS)[3,6,7] has been implemented into Nastcomb. The model is suitable to interpreting, in addition to predicting, a series of important physical phenomena taking place in turbulent fluctuating-property flow fields. Quite importantly, this result has been obtained without inducing an overwhelming increase in computing demands. The TSDIA/MTS approach operates in the ensemble-mean space rather than in the favre-averaged one: adopting this procedure, several correlations arise and must be modeled. The final results are synthesised by the following closures:

$$\begin{aligned}-<u_i'u_j'>+\frac{2}{3}K\delta_{ij}&=\nu_{TC}S_{ij}-\frac{3}{4}\frac{\nu_{TC}^2}{K}\left[S_{ik}S_{kj}+S_{jk}S_{ki}\right]_D+\\&-\frac{3}{4}\frac{\nu_{TC}^2}{K}\left[S_{ik}\Omega_{kj}+S_{jk}\Omega_{ki}\right]\end{aligned} \tag{4}$$

$$\text{where}\quad \Omega_{ij}=\frac{\partial U_j}{\partial x_i}-\frac{\partial U_i}{\partial x_j} \tag{5}$$

with $\left[N_{ij}\right]_D=N_{ij}-\frac{1}{3}N_{hh}\delta_{ij}$, the deviatoric part of the (generic) tensor N_{ij}.

The variable-density counterpart ν_{TC} of the incompressible eddy viscosity ν_{TS} turns out of the form:

$$\nu_{TC}=\frac{\nu_{TS}}{\left[1+A\left(K_{\rho N}/M_T^2\right)\right]^{3/2}}=\frac{C_\nu K^2/\varepsilon}{\left[1+A\left(K_{\rho N}/M_T^2\right)\right]^{3/2}} \tag{6}$$

with $K_{\rho N}=\left\langle\rho'^2\right\rangle/\overline{\rho}^2$ the normalized density variance accounting for compressibility effects, and with $M_T=\sqrt{\left\langle\mathbf{u}'^2\right\rangle}/\overline{a}=\sqrt{2K/[\gamma(\gamma-1)E]}$ the turbulent Mach number.

From eq.(6) it can be noticed that compressibility lowers the eddy-viscosity as it tends to smooth out velocity fluctuations and dissipating turbulence energy. Transport equations

for the turbulent kinetic energy (K), for its dissipation rate (ε) and for the density-variance are given below:

$$\bar{\rho}\frac{DK}{Dt} = -\bar{\rho} < u_i' u_j' > \frac{\partial U_i}{\partial x_j} - \bar{\rho}\varepsilon\left(1 + \frac{1}{\bar{\rho}\varepsilon} < \rho'\mathbf{u}' > \cdot\frac{D\mathbf{U}}{Dt}\right) + \nabla\cdot\left[\left(\bar{\rho}\frac{\nu_{TS}}{\sigma_K} + \bar{\mu}\right)\nabla K\right] \tag{7}$$

$$\bar{\rho}\frac{D\varepsilon}{Dt} = -C_{\varepsilon 1}\frac{\varepsilon}{K}\bar{\rho} < u_i' u_j' > \frac{\partial U_i}{\partial x_j} - C_{\varepsilon 2}\bar{\rho}\frac{\varepsilon^2}{K} + \nabla\cdot\left[\left(\bar{\rho}\frac{\nu_{TS}}{\sigma_\varepsilon} + \bar{\mu}\right)\nabla\varepsilon\right] \tag{8}$$

$$\frac{DK_\rho}{Dt} = -2 < \rho'\mathbf{u}' > \cdot\nabla\bar{\rho} - 2K_\rho\nabla\cdot\mathbf{U} - C_D\left(1 + A\frac{K_{\rho N}}{M_T^2}\right)^{3/2}\frac{\varepsilon}{K}K_\rho + \nabla\cdot\left(\frac{\nu_{TS}}{\sigma_{\rho\rho}}\nabla K_\rho\right) \tag{9}$$

The constants have been, as of now and tentatively, assigned the following values:

$$\begin{aligned} &C_\nu = 0.09 \quad \sigma_e = 1.0 \quad \sigma_K = 1.0 \quad \sigma_{\rho\rho} = 1.0 \quad \sigma_\rho = 2.0; \\ &\sigma_\varepsilon = 1.3 \quad C_{\varepsilon 1} = 1.44 \quad C_{\varepsilon 2} = 1.92 \quad C_D = 0.3 \quad A = 5 \end{aligned} \tag{10}$$

The TSDIA/MTS expressions for the density-velocity correlation and for energy-velocity correlation (turbulent energy flux) are respectively:

$$< \rho'\mathbf{u}' > = -\frac{\nu_{TC}}{\sigma_\rho}\nabla\bar{\rho} - \frac{3}{2}(\gamma - 1)\nu_{TC}\frac{\bar{\rho}}{K}K_{\rho N}\nabla E \tag{11}$$

$$< e'\mathbf{u}' > = -\frac{\nu_{TC}}{\sigma_\mathbf{e}}\nabla E \tag{12}$$

Combustion simulation is performed following a "partial-equilibrium" approach[3], whereby all reactions are pre-partitioned in two groups, the "slow" ones, which proceed kinetically (Arrhenius kinetics assumed), and the "fast" reactions, assumed in equilibrium at all times. This approximation greatly reduces the numerical problems induced by the stiffness of the system of equations governing the time-evolution of the species concentrations. A so-called quasi-global scheme has been developed[6], in which an overall methane partial-oxidation step is assumed as:

$$2\mathrm{CH_4} + \mathrm{O_2} = 2\mathrm{CO} + 4\mathrm{H_2} \tag{13}$$

Its rate ω_{ov}, obtained through calibration, turns out the following:

$$\omega_{ov} = 5.635\cdot 10^5\cdot\exp\left(-\frac{30.0}{RT}\right)\cdot[\mathrm{CH_4}]^{0.25}\cdot[\mathrm{O_2}]^{0.715} \tag{14}$$

This overall reaction is adjoint by a set of 5 equilibrium and 7 kinetic elementary-reactions. The species considered are : CH_4, O_2, O, CO, CO_2, H_2, H_2O, H, OH, N_2, N, NO. In order to take care of turbulence effects we write[7] the rate of change of mass fraction as:

$$\frac{dY_m}{dt} = -\frac{\left(Y_m - Y^*\right)}{\tau_c} \tag{15}$$

where Y_m is mass fraction of species m , Y^* is local and instantaneous thermo-dynamic equilibrium value of mass fraction, and τ_c is characteristic time to achieve such equilibrium. This time is assumed the same for all species (less nitrogen). The expression of τ_c is evaluated as the sum of a molecular time-scale τ_l and a turbulent time-scale τ_t :

$$\tau_c = \tau_l + f\,\tau_t \tag{16}$$

where the delay coefficient f can be taken as unit, no assumption of reaction completeness being imposed. The molecular time-scale is that given by the quasi-global reaction eq.(14):

$$\tau_l = \left(5.635 \cdot 10^5\right)^{-1} \cdot \exp\left(+\frac{30.0}{RT}\right) \cdot [CH_4]^{0.75} \cdot [O_2]^{0.715} \tag{17}$$

The turbulent time-scale τ_t is proportional to the eddy turnover time:

$$\tau_t = C\frac{k}{\varepsilon} \tag{18}$$

with $C = 0.10$, i.e. the same value given by the RNG k-ε model.

In Nastcomb's latest version an advanced, nonequilibrium, continuous-field, time-dependent 3D radiation model has been introduced[8], and made interactive with the thermo-fluid-dynamical and combustive solution. Originally the model, of “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[9,10]. In synthesis, the transport equation for the radiation energy-density E_r is written as:

$$\frac{\partial E_r}{\partial t} + \nabla \cdot \overline{F_r} = \frac{c}{\rho_g}(aT_g{}^4 - E_r) \tag{19}$$

where T_g is the gas temperature, $\overline{F_r}$ is the radiation flux vector, ρ_g is the gas density, "c" is the speed of light, and "a" is the radiation constant (7.653 e-15 erg/cm^3 K^4). Eq.(19) is solved together with the gas energy-density equation:

$$\frac{\partial(\rho E)_g}{\partial t} = -\frac{c}{\rho_g}(aT_g{}^4 - E_r) \tag{20}$$

The coupling terms which relate the radiation energy density E_r to the fluid energy density E are large when the photon mean-free paths, due to molecular collisions, are small ("optically-thick" regions).

The i-th component of the radiation flux vector $\overline{\mathrm{F}}_{\mathrm{r}}$ is given by:

$$F_i = -f_i \frac{c\lambda_g}{3} (\nabla E_r)_i \tag{21}$$

where the mean-free path λ_{g} is the total one, i.e. inclusive of absorption and scattering. The flux limiting functions $\mathrm{f_i}$ have the expression:

$$f_i = \frac{1}{1 + g_i \left[1 + 3\exp\left(-\frac{3}{2} g_i \right) \right]} \tag{22}$$

where :

$$g_i = \frac{1}{3} \frac{\lambda_g}{E_r} \left| (\nabla E_r)_i \right| \tag{23}$$

Notice that when $\mathrm{g_i} << 1$, $\mathrm{f_i} \approx 1$, and F_i represents a conventional diffusive flux of E_r along the i-th direction. When $\mathrm{g_i} >> 1$, $\mathrm{f_i}$ becomes very small ("optically-thin" regions) and flux limiting occurs, so to satisfy the constraint (upon max radiation flux) given by the product of light speed and energy-density.The values of λ_{g} are evaluated through the formulation:

$$\lambda_g = \frac{-L}{\ln(1 - \varepsilon_g)} \tag{24}$$

where the characteristic length L is taken as: 3.5 x (volume)/(wall-surface area). The parameter ε_{g} is a gray-medium emissivity for the gas, evaluated by assuming that the dominant radiative absorbers/scatterers are H_2O and CO_2 .

Coupled equations (19,20) are solved in implicit finite difference form: the values of gas internal energies E are so updated at the beginning of each time step, and are then introduced into energy equation (3) in order to take care, in this way, of the radiation effects Q_{rad}.

Once the flow-field is numerically discretised and the proper boundary conditions are defined, the net exchange $q_{w,g}$ in the energy-radiation process between a fluid-cell and a wall-cell is given by:

$$q_{w,g} = const \left(\varepsilon_g T_g^4 - \alpha_g q_w \right) \tag{25}$$

where α_g is the gas absorptivity and q_w is the total heat flux leaving the wall (radiosity), which is given by:

$$q_w = (1 - \varepsilon_w) \varepsilon_g T_g^4 + \varepsilon_w T_w^4 \tag{26}$$

The gas absorptivity α_g is related to the emissivity ε_g through:

$$\alpha_g = \varepsilon_g \left(\frac{T_g}{T_w} \right)^{(0.6-0.2\,\xi)} \tag{27}$$

where T_g is the mixture temperature, T_w is the temperature of the incoming radiation source (emitter), and ξ describes the local concentration of water vapor and carbon dioxide as:

$$\xi = \frac{p_{H_2O}}{\left(p_{H_2O} + p_{CO_2} \right)} \tag{28}$$

We thus obtain:

$$q_{w,g} = \left(\frac{A_w \cdot \sigma \cdot \Delta t \cdot F_{w,g}}{vol_g} \right) \cdot \left[\varepsilon_g T_g^4 - \alpha_g \left(1 - \varepsilon_w \right) \varepsilon_g T_g^4 - \alpha_g \varepsilon_w T_w^4 \right] \tag{29}$$

where Δt is time-step, σ is Stefan-Boltzmann constant, A_w is wall surface and vol_g is fluid-cell volume. $F_{w,g}$ is the fraction of energy leaving the wall surface which reaches the fluid-cell (radiation shape factor), which can be approximately evaluated as:

$$F_{w,\,g} \;\approx\; cos\beta_2 \tag{30}$$

where the angle β_2 is measured between the normal to the surface and the line drawn from the center of the fluid-cell to the center of the wall-cell.

CONCLUSIONS

In this Part I of the paper, a wide-breadth numerical strategy has been presented, which appears suitable to treat complex problems, such as those related to combined fluid-dynamical and thermo-chemical fields, starting from fundamentals (instead of directly going into more sophisticated modelisations), and identifying, from a physics point of view, the real "causes" acting upon the respective end-effects. In other words, the basic presumption of the study is that a more deep interpretation of general mechanisms (e.g. radiation heat transfer, turbulence basic behavior, physical boundary conditions, etc.) would succeed far better than an updated "calibration" of some coefficients: the outcome of Part II will prove this point.

The overall solution strategy for the 3D compressible Navier-Stokes equations, suitable for turbulent reacting flows, here discussed can be considered as a valid alternative to the pervasive offer of so-called multi-purpose codes, in this field, coming from commercial software houses. Quite peculiarly, the solver Nastcomb, under development at DIMSET for more than ten years, though very general in its applicability range, responds to a logic of “specific-purpose” code. This means that, as the listed references attest, given a particular application, a specialised version of the code either exists or can be set up, specifically tailored and validated upon that case, so to yield a pre-assessment of the expected accuracy and reliability of predictions.

Within this perspective, the theoretical research here discussed has succeeded in performing both the numerical configuration and then also the experimental validation of a very specific version of solver Nastcomb, namely that to be adopted, on ground of its advanced physical models, and specifically of the radiation model, for applications to burners and combustors operating with premix-flames of natural-gas in air. So to say, the validation procedure has thus become instrumental to a “targeted” configuration of the solver. The target being the achievement of a level of "theoretical reliability" competitive with the direct experimentation.

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