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DNS/CAA ANALYSIS OF THE SOUND FIELD RADIATED FROM A TURBULENT PREMIXED FLAME

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Abstract
A hybrid DNS/CAA method is used in this work to analyze acoustic wave emission and propagation caused by thermoacoustic sources. The numerical approach is a two-step method, the first step of which is based on a Direct Numerical Simulation (DNS), followed by the computational aeroacoustics (CAA) step using the acoustic perturbation equations for reacting flows (APE-RF). A CO/H_2/Air turbulent premixed flame is investigated by a fully compressible DNS code. Chemical processes are computed using a complete reaction scheme and accurate transport properties are taken into account. The DNS results have been interpolated onto the CAA grid via a multi-linear algorithm. to evaluate the source terms of the APE-RF system. Using a detailed description of the flow based on the DNS solution, an extensive analysis of the sources in terms of the radiated acoustic field is possible. Within this work it will be shown that acoustic simulations of turbulent flames can be performed using the total time derivative of the density instead of the unsteady heat release rate. Moreover, the capability of the DNS simulations to deliver the appropriate source term of the APE-RF system will be presented.

INTRODUCTION

A hybrid DNS/CAA method is proposed in this work to investigate in detail the noise radiated from a turbulent premixed CO/H_2/Air flame. Noise generated and radiated from a turbulent

flame has been mainly predicted in the past through computations of inhomogeneous wave equations using an ordinary wave operator [1, 2]. Recently, Bui et al. [3] presented a hybrid method to simulate acoustic wave propagation generated by thermoacoustic sources. Their results were based on large-eddy simulations (LES) and acoustic perturbation equations (APE) extended to reacting flows (RF). The acoustic simulations have been performed using the total time derivative of the density as major source term instead of the unsteady heat release rate, since the latter was not directly available from the LES. Using the DNS solution we are able to compare the acoustic impact of the total time derivative of the density and the unsteady heat release rate as major source term.
The DNS code employed for this study, called *parcomb*, has initially been developed by Thévenin et al. and has been described in detail in [5, 6]. The DNS results can be seen as a kind of "numerical experiment", since numerical diffusion is kept below the level of physical diffusion. The evolution of turbulence is thus only given by the Navier-Stokes equations and not by any approximate turbulence model.
In this paper we will in particular try to answer following questions:

- Is DNS able to deliver detailed information to evaluate the sources of the APE-RF system?
- Is the acoustic field associated with turbulent reacting flows equally described by the total time derivative of the density instead of the unsteady heat release rate?

ACOUSTIC PERTURBATION EQUATIONS FOR REACTING FLOWS

The acoustic radiation of the aforementioned premixed flame is simulated by solving the acoustic perturbation equations for reacting flows (APE-RF). They read

$$\frac{\partial \rho'}{\partial t} + \nabla \cdot \left(\rho' \overline{\boldsymbol{u}} + \overline{\rho} \boldsymbol{u}' \right) = q_{c,rf} \tag{1}$$

$$\frac{\partial \boldsymbol{u}'}{\partial t} + \nabla \left(\overline{\boldsymbol{u}} \cdot \boldsymbol{u}' \right) + \nabla \left(\frac{p'}{\overline{\rho}} \right) = \boldsymbol{q_{m,rf}} \tag{2}$$

$$\frac{\partial p'}{\partial t} - \overline{c}^2 \frac{\partial \rho'}{\partial t} = q_{e,rf} \tag{3}$$

while the sources of which are

$$q_{c,rf} = -\nabla \cdot \left(\rho' \boldsymbol{u}' \right)' \tag{4}$$

$$\begin{aligned} \boldsymbol{q_{m,rf}} = & -\left(\boldsymbol{\omega} \times \boldsymbol{u} \right)' - \left(\nabla \frac{(u')^2}{2} \right)' + \left(\frac{\nabla \cdot \tau}{\rho} \right)' + T' \nabla \overline{s} - s' \nabla \overline{T} + \left(\sum_n Y_k \boldsymbol{f}_k \right)' \\ & + \left(\sum \left(\frac{\mu_k}{M_k} \right)' \cdot \nabla \overline{Y_k} \right) - \left(\sum Y_k' \cdot \nabla \overline{\left(\frac{\mu_k}{M_k} \right)} \right) \end{aligned} \tag{5}$$

$$
\begin{aligned}
q_{e,rf} \;=\; & -\overline{c}^2 \left[\frac{\overline{\rho}}{\rho} \cdot \frac{\alpha}{c_p} \cdot \left(\sum_{n=1}^{N} \left. \frac{\partial h}{\partial Y_n} \right|_{\rho,p,Y_m} \rho \frac{DY_n}{Dt} + \nabla \cdot \boldsymbol{q} - \frac{\partial u_i}{\partial x_j} \tau_{ij} \right) \right. \\
& -\nabla \cdot (\boldsymbol{u} \rho_e) - \frac{1}{\overline{c}^2} \left[\left(1 - \frac{\overline{\rho c^2}}{\rho c^2} \right) \cdot \frac{Dp}{Dt} - \frac{p - \overline{p}}{\rho} \cdot \frac{D\rho}{Dt} \right] \\
& \left. + \left[-\frac{\gamma - 1}{\gamma} \boldsymbol{u} \cdot \nabla \overline{\rho} \; - \frac{p}{\overline{c}^2} \cdot \boldsymbol{u} \left(\frac{\nabla \overline{p}}{\overline{p}} - \frac{\nabla \overline{\rho}}{\overline{\rho}} \right) \right] \right]. \qquad (6)
\end{aligned}
$$

The APE-RF system is based on the homogeneous APE system developed by Ewert and Schröder [7]. For combustion noise simulations this homogeneous system has been chosen to take advantage of its benign properties to simulate wave propagation, i.e., its validity for non-uniform mean flows, while excitations of instabilities are prevented. To derive the APE-RF system, the governing equations for reacting flows are rearranged such that the left-hand side describes the original homogeneous APE system [7], whereas the right-hand side (RHS) consists of all non-linear flow effects including the sources related to chemical reactions. When combustion noise at low Mach numbers is considered, the major source term can be found within the sources of the pressure-density relation $q_{e,rf}$, i.e., the entropy fluctuations due to non-isentropic processes during combustion.

It is well known from theoretical investigations [2] that the unsteady heat release rate is the dominant acoustic source term when reacting flows are considered. Bui et al. showed in [3] that using the total time derivative of the density as major source term the simulated radial acoustic intensity of turbulent diffusion flames is in good agreement with experimental data. The source terms within the RHS of the APE-RF system can be evaluated from unsteady CFD solutions of the reacting flow such as LES or DNS. However, using DNS results, the sources especially including chemical reacting flow effects can be evaluated in detail since full reaction schemes are taken into account. The expression for the total time derivative of the density can be derived using the energy equation for reacting flows

$$
\frac{D\rho}{Dt} \;=\; \frac{1}{c^2} \frac{Dp}{Dt} + \frac{\alpha}{c_p} \cdot \left(\sum_{n=1}^{N} \left. \frac{\partial h}{\partial Y_n} \right|_{\rho,p,Y_m} \rho \frac{DY_n}{Dt} + \nabla \cdot \boldsymbol{q} - \frac{\partial u_i}{\partial x_j} \tau_{ij} \right), \qquad (7)
$$

As was shown in detail in [3], the total time derivative consists besides the unsteady heat release rate of several other source mechanisms. The effect of non-isomolar combustion, the effects of mass and heat diffusion, and a term describing the influence of viscous flow effects occur in the total rate of change of the density with respect to time.

PROBLEM DEFINITION

The numerical domain under investigation is a square box of dimension L=1.2x1.2 cm^2 as shown in Figure 1(a). A fixed mesh of 355 points is used in each direction. This leads to a spatial resolution of 33 μm, necessary to resolve intermediate radicals. The left-hand boundary condition is a subsonic inlet at an imposed inlet velocity of 1 m/s, while on the right-hand boundary a non-reflecting subsonic outlet condition is formulated. A complete reaction

scheme with 13 species (CO, HCO, CH_2O, CO_2, H_2O, O_2, O, H, OH, HO_2, H_2O_2, H_2, N_2) and 67 individual reactions is taken into account. First, the corresponding premixed laminar flame is computed for a one-dimensional flow along the x-direction and the inlet velocity is adapted to keep the flame front in the center of the domain. Then, the obtained steady solution is transposed to a 2-D flow, with fresh gases on the left side and burnt gases on the right side. An isotropic 2-D turbulent velocity field is superposed using a von Kármán spectrum coupled with Pao correction for near-dissipation scales [6, 8, 9].

NUMERICAL METHODS

Direct Numerical Simulation

The simulation presented here has been carried out using *parcomb* code developed by Thévenin et al. [5, 6]. It is a finite-difference DNS code solving the compressible Navier-Stokes equations for multicomponent reacting flows. Derivatives are computed using sixth order approximations except at boundaries where the discretization is fourth order. The temporal integration is realized by a 4-stage Runge-Kutta algorithm of order four. Boundary conditions are formulated using the Navier-Stokes Characteristic Boundary Condition (NSCBC) technique [10], extended to take into account multicomponent thermodynamic properties [11]. Transport coefficients and chemical kinetics are treated similar to both methods used in CHEMKIN II and TRANSPORT [12, 13]. The DNS code has been parallelized and widely used over the last ten years to investigate turbulent flames[6, 8, 14]. *Parcomb* has already been validated for H_2-O_2-N_2 premixed flame velocities of various composition. Many experimental results are available for this problem. The very good agreement between experimental and computed values is evidenced in Figure 1(b). Having gained confidence in the code, we now illustrate its possibilities to deliver detailed information to determine the sources of the APE-RF system.

CAA computation

Since the source terms are calculated on the DNS grid, which does not coincide with the acoustics mesh, they need to be interpolated onto the CAA grid. This is done via a trilinear algorithm. The CAA computation is performed on a 9-block mesh with 300x300 grid points. During the CAA computations the source terms on the RHS of the APE-RF system are interpolated in time. For this purpose, a quadratic interpolation method is used, which requires at least 25 points per period to achieve a sufficiently accurate distribution. The CAA code is based on the fourth-order dispersion-relation preserving (DRP) scheme of Tam and Webb [16] for the spatial discretization and the alternating low-dissipation low-dispersion Runge Kutta (LDDRK) method in the 5/6 mode for the temporal integration by Hu et al. [17]. At the far-field boundaries the radiation boundary condition by Tam et al. [16] is used to avoid unphysical backscatter into the computational domain. For the CAA computations, mean flow effects are neglected and combustion at constant pressure is assumed.

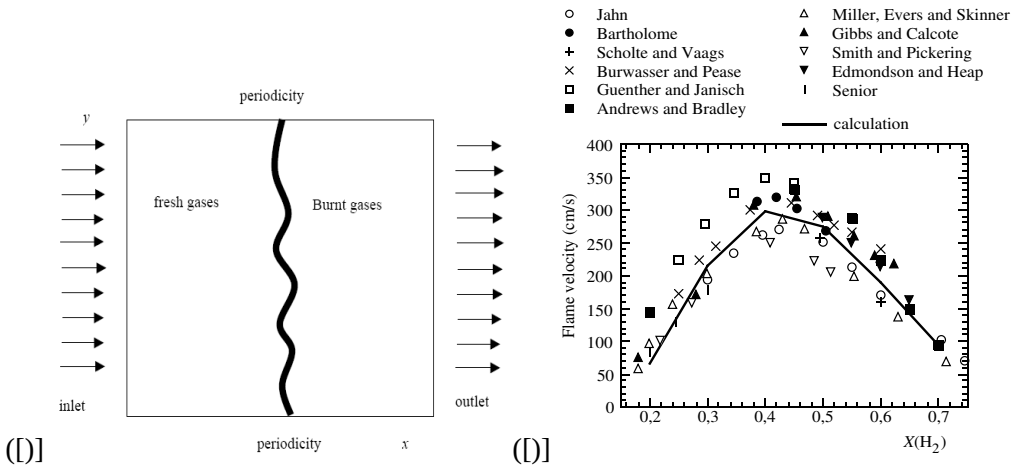

Figure 1: Numerical configuration employed for the DNS (a), comparison of experimental and computed $H_2 - O_2 - N_2$ flame velocities (b). References of the experimental results are listed in [15]

RESULTS AND DISCUSSIONS

Flow field

The typical temporal evolution of the premixed flame is shown in Figure 2. To visualize the structure the instantaneous heat release rate has been chosen. The flame front gets strongly stretched and curved by interacting with the turbulence field, leading to considerable modifications of the heat release field up to almost local extinctions. In Figure 3 the spatial distri-

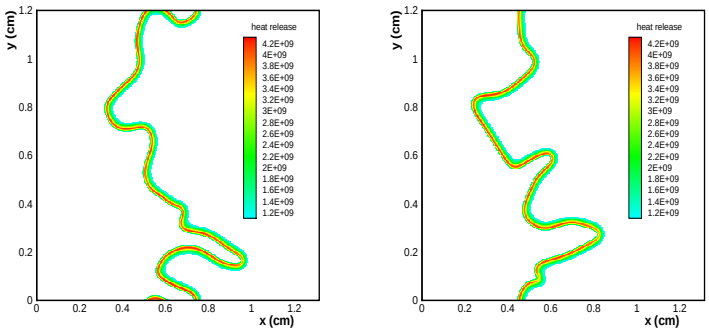

Figure 2: Instantaneous spatial distribution of heat release in a premixed CO/H_2/Air flame after interacting with a turbulent velocity field for $t = 1.0$ ms (left) and $t = 1.5$ ms (right)

butions of the H_2O_2 and HO_2 mass fraction after an interaction duration of $t = 1.0$ ms are presented. It can be noted that the variations along the flame front are rather small due to the

relatively low turbulence level of the flame under consideration.

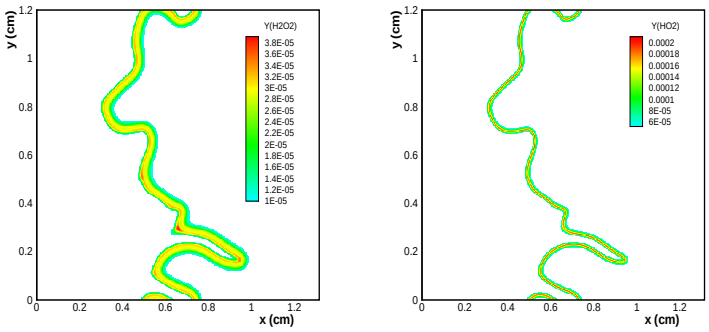

Figure 3: Instantaneous spatial distribution of H_2O_2 and HO_2 mass fractions in a premixed CO/H2/Air flame after interacting with a turbulent velocity field for $t = 1.0$ ms

CAA results

The directivity patterns are evaluated for different frequencies from 180 observer points uniformly distributed on a circle with a non-dimensional radius of $R/L = 2.2$. The origin of which coincides with the center of the DNS domain and the CAA domain. The directivity patterns in Figure 4 evidence the dominant part of the simulated acoustic field, which is characterized by the low frequencies, to be of monopole type and of the same order of magnitude for both simulations. That is, the distributions based on the substantial time derivative of the density or the unsteady heat release rate as major source term do coincide. The differences in the higher frequency range shown in Figures 4(d) and 4(h) could be attributed to the additional sources that are included within the total time derivative of the density[4].

CONCLUSIONS

When combustion noise is analyzed, the heat release represents the main source term in the APE-RF system. However, the heat release can also be expressed via the total time derivative of the density. Comparing the acoustic field of turbulent flames it can be concluded for frequencies containing the major acoustic energy content that the total time derivative of the density can be used instead of the unsteady heat release rate. The differences observed in the directivity patterns in the higher frequencies range between the substantial time derivative of the density and the heat release rate could be attributed to the additional sources included only within the total time derivative of the density. This question will be addressed in future work.

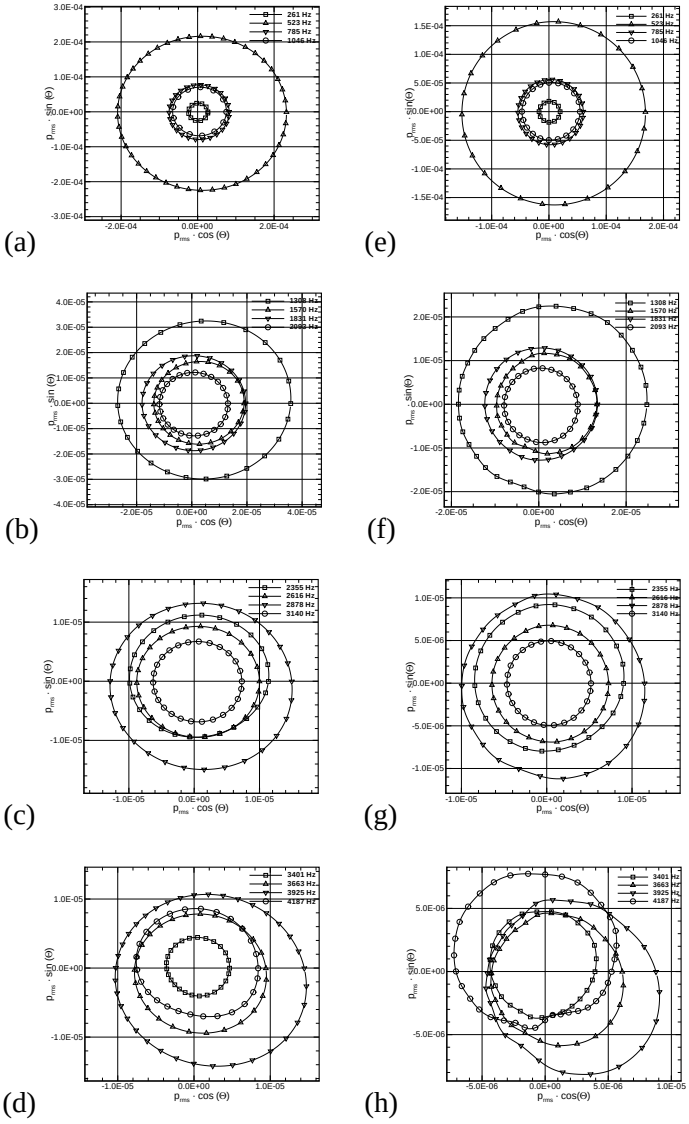

Figure 4: Directivity patterns for different frequencies; comparison of the unsteady heat release rate (a-d) or the total time derivative of the density (e-h) as major source term

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