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Numerical analysis of the acoustics of a diffusion flame

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ABSTRACT

The aim of this work is to obtain an analytical–numerical solution for a jet diffusion flame in a closed domain and analyze its acoustic field. The combustion chamber is a closed three-dimensional region in which a jet of methane is injected separated from the jet of air. To analyze the influence of the flame under the acoustic field, two tests are performed: in the first test occurs only the mixing, and in the second test occurs the mixing and the chemical reactions. The proposed model uses the Navier–Stokes, mass conservation and wave equations, which are solved numerically. The flow equations are coupled with the equations for the mass fraction of chemical species and temperature, which are solved analytically based on the flamelet model. The numerical scheme follows the finite difference method and the Runge–Kutta multistage scheme is employed for the integration in time. An estimate for the error is presented based on the solution of three grids using the error estimator of Richardson. The results show good agreement with data from the literature. The proposed model is a quick and less expensive option to investigate the acoustic field of reactive flows in a closed region.

1. Introduction

Combustion is present in many kinds of industries such as in aviation, production of iron, and transformation of energy. Gas turbines are a common example of the use of combustion in industry. In developing these equipments many problems should be anticipated such as flashback, quenching and oscillations of the combustion. These devices work with high rates of energy conversion and it is important that the flame remains stable even in the presence of turbulence. Any instability can blow out the flame or increase the pollutants production such as nitrous oxides.

The thermoacoustic coupling can generate oscillations in pressure, which may increase with time due to feedback caused by the release of heat and the interaction with the walls of the combustion chamber. The pressure variations also produce vibration in the combustion chamber and these vibrations can decrease the lifetime of the equipments. Therefore, an efficient control of this process allows a cheaper and safer operation. However, combustion is a complex physical phenomenon that involves many factors that influence each other.

Rayleigh [1] employed equivalent sources to describe the acoustic behavior of a non-uniform flow in free space. Lighthill [2] employed the same idea for the development of an analogy in which the equations of motion of the fluid, expressed as the conservation of mass and movement, were combined to obtain a wave equation with nonlinear source terms. The set of equations of Lighthill describes the nonlinear generation of sound for an unstable flow, not considering the radiation effect away from its source.

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Other authors, such as Curle [3], Ffowcs and Hawkings [4], had made changes in the acoustic analogy to describe the influence on the flow due to the contours. To describe the influence of physical processes some authors use a change of variable in the wave equation, which allows to analyze other characteristics of the flow. Morfey [5], Lilley [6] and [7] used as variable the pressure, Ffowcs [8] and Kambe [9] used the variable $p + \rho u^2/3$, where p is the pressure, ρ is the density and $\mathbf{u}$ is the velocity. Howe [10] uses the enthalpy of the stagnation. Goldstein [11–13] discussed a number of extensions of the original concept proposed by Lighthill [2].

To investigate the acoustics of a flame it is necessary to consider various characteristics such as the type of flow (laminar or turbulent), type of flame (diffusive or premixed) and fuel type. In this paper, a turbulent diffusion flame of methane inside a combustion chamber is considered. The equations of Navier–Stokes for Large-Eddy Simulation are used to obtain the velocity field coupled with the equations that describe the reaction of methane combustion and the wave equation, to consider the pressure variation generated by the turbulent flow. These equations are solved numerically using the finite difference scheme with a fourth-order approximation in space and third order in time. An analytical solution for diffusion of the chemical species and the temperature is presented. Numerical tests are carried out in a 3D rectangular combustion chamber where the fuel is injected in the left side and the products of combustion are free to leave the chamber in the right side of the chamber.

In the next section the equations of the problem are presented. The formulation is based on the flamelet model and the acoustic perturbation equations proposed by Bui [14]. Section 3 presents an analytical solution for the equations of the flamelet model. Section 4 describes the methods used to approximate the spacial derivative and the temporal integration based on the Runge–Kutta method. In Section 5 the results obtained for the methane burning inside a combustion chamber are presented. After that, we present the results and their discussion, followed by the conclusions.

2. Governing equations

In the following, the acoustic field generated by the non-premixed burning of methane with air in the combustion chamber is modeled. The flow is considered compressible and turbulent. The chemical reaction is given by two equations that relate 5 chemical species as proposed by Roux [15]

$$\mathrm{CH_4} + \frac{3}{2}\mathrm{O_2} \rightarrow \mathrm{CO} + 2\mathrm{H_2O}, \tag{1}$$

$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \rightleftarrows \mathrm{CO_2}. \tag{2}$$

Their reaction rates are given by, respectively:

$$q_1 = A_1 \left(\frac{\rho Y_{\mathrm{CH_4}}}{W_{\mathrm{CH_4}}}\right)^{n_{1F}} \left(\frac{\rho Y_{\mathrm{O_2}}}{W_{\mathrm{O_2}}}\right)^{n_{1O}} \exp\left(-\frac{E_{a1}}{RT}\right), \tag{3}$$

$$q_2 = A_2 \left[\left(\frac{\rho Y_{\mathrm{CO}}}{W_{\mathrm{CO}}}\right)^{n_{2\mathrm{CO}}} \left(\frac{\rho Y_{\mathrm{O_2}}}{W_{\mathrm{O_2}}}\right)^{n_{2O}} - \left(\frac{\rho Y_{\mathrm{CO_2}}}{W_{\mathrm{CO_2}}}\right)^{n_{2\mathrm{CO}}}\right] \exp\left(-\frac{E_{a2}}{RT}\right), \tag{4}$$

where $A_1 = 2 \times 10^{15}$, $A_2 = 2 \times 10^9$, $n_{1F} = 0.9$, $n_{1O} = 1.1$, $n_{2\mathrm{CO}} = 1$, $n_{2O} = 0.5$, $E_{a1} = 35{,}000$ and $E_{a2} = 12{,}000$.

Eqs. (1) and (2) are a simplification for the process of oxidation of methane which has dozens of chemical species. Nevertheless, the direct use of Eqs. (1) and (2) in the model implies a high computational cost because the implementation of a convective–diffusive equation for each chemical species is required. In addition, the time scale of the reactions is very small. Therefore, to reduce the computational cost of the chemical problem, the *mixture fraction* (Z ranging from 0 to 1) is introduced:

$$Z = \frac{\nu Y_F - Y_{\mathrm{O_2}} + Y_{\mathrm{O_2}}^{in}}{\nu Y_F^{in} + Y_{\mathrm{O_2}}^{in}} \tag{5}$$

where ν is the stoichiometric mass ratio, Y_F is the local mass fraction of the Fuel, Y_F^{in} is the initial mass fraction of the Fuel, $Y_{\mathrm{O_2}}$ is the local mass fraction of the oxidizer and $Y_{\mathrm{O_2}}^{in}$ is the initial mass fraction of the oxidizer.

It is assumed that the flame occurs when Z reaches its stoichiometric value. This value can be calculated by:

$$Z_{st} = \left(1 + \frac{\nu Y_F^{in}}{Y_{\mathrm{O_2}}^{in}}\right)^{-1}. \tag{6}$$

The set of equations can be transformed from the physical space to the mixture fraction space using the transformations:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial Z} + \frac{\partial Z}{\partial t}\frac{\partial}{\partial Z} \tag{7}$$

$$\frac{\partial}{\partial x_k} = \frac{\partial}{\partial Z_k} + \frac{\partial Z}{\partial x_k}\frac{\partial}{\partial Z}. \tag{8}$$