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An efficient flamelet-based combustion model for compressible flows

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ABSTRACT

A combustion model based on a flamelet/progress variable approach for high-speed flows is introduced. In the proposed formulation, the temperature is computed from the transported total energy and tabulated species mass fractions. Only three additional scalar equations need to be solved for the combustion model. Additionally, a flamelet library is used that is computed in a pre-processing step. This approach is very efficient and allows for the use of complex chemical mechanisms. An approximation is also introduced to eliminate costly iterative steps during the temperature calculation. To better account for compressibility effects, the chemical source term of the progress variable is rescaled with the density and temperature. The compressibility corrections are analyzed in an *a priori* study. The model is also tested in both Reynolds-averaged Navier–Stokes (RANS) and large-eddy simulation (LES) computations of a hydrogen jet in a supersonic transverse flow. Comparison with experimental measurements shows good agreement, particularly for the LES case. It is found that the disagreement between RANS results and experimental data is mostly due to the mixing model deficiencies and the presumed probability density functions used in the RANS formulation. A sensitivity study of the proposed model shows the importance of the compressibility corrections especially for the source term of the progress variable.

1. Introduction

As part of the renewed interest in high-speed flight, a need was identified for the development of hypersonic air-breathing propulsion systems using ambient air as oxidizer. These systems have long been recognized as the most well-suited for hypersonic propulsion. Although a traditional ramjet is most appropriate in the supersonic regime (Mach 3–5), hypersonic speeds (Mach 6–15) can be reached only with the use of a scramjet, where combustion takes place at supersonic speeds. Because of the high speed in scramjet combustors, the flow has a very short residence time inside the engine, during which air and fuel must mix on a molecular level, and chemical reactions have to be completed. Although some ground and flight experiments have successfully demonstrated the feasibility of supersonic combustion [1–4], experimental testing requires a large investment and presents numerous difficulties. Computational tools are thus a key element toward the development of an efficient, high-performance scramjet engine, and because mixing and heat release are at the heart of a scramjet operation, the development and use of accurate combustion models for supersonic combustion are critical.

The vast majority of computational modeling work in supersonic turbulent combustion so far has relied on simplified/reduced chemical mechanisms and the explicit transport of the involved species [5]. Such approaches require the closure for the filtered (or ensemble averaged) chemical source term in the species transport equations. This can be achieved, for example, with simpler but low-accuracy models such as the direct use of the Arrhenius law with the mean quantities [6,7], which neglects closure, the Eddy Dissipation Concept model [8], or with closure based on assumed [9,10] or transported [11–14] probability density functions (PDF). Also, the Linear Eddy model (LEM) [15,16] has been applied for this case. However, due to the strong non-linearity of the source term and the wide range of time scales associated with the chemistry, reactive transport equations are very stiff and difficult to solve. Moreover, due to very short residence times in high speed flows, flame stabilization mechanisms are often governed by auto-ignition. It is critical to model accurately such ignition and extinction phenomena in order to predict the stability of scramjet combustion. Therefore, an approach based on detailed chemical kinetics, which can predict flame stabilization, is required. While a model transporting all involved species can easily be extended to more

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detailed chemical mechanisms, it quickly becomes computationally intractable, especially when complex fuels must be considered.

An alternative approach is based on the flamelet concept [17,18], which assumes that the chemical time scales are shorter than the turbulent time scales so that the flame can be approximated as an ensemble of laminar flamelets. The so-called steady flamelet approach allows the computation of the chemistry to be performed independently of the flow simulation and stored in tabulated form as a function of a limited number of scalars. During the actual simulation, the quantities of interest are read and interpolated, thus, dramatically decreasing the computational cost and allowing the use of complex chemical mechanisms. In the low Mach number flamelet implementation, the temperature and the species mass fraction are assumed to depend only on two scalars, traditionally the mixture fraction and its dissipation rate. Chemical tables are then constructed assuming constant background pressure. This formulation can also be extended to better reproduce the unsteady character of combustion by replacing the scalar dissipation rate with a progress variable [19,20].

The typical implementation of the flamelet model is based on a low Mach number assumption, explaining the still very limited number of studies of high-speed flows using this approach [21–23]. Kumar and Tamaru [23] used a laminar flamelet model to simulate a compressible ram combustor, where the temperature was interpolated from a flamelet library based on the mixture fraction and scalar dissipation rate. Oevermann [22] extended this model by computing the temperature from the internal energy and the species mass fractions, where the energy is determined from the solution of a transport equation, and the species mass fractions were interpolated from a flamelet table, based on the same parameters and without introducing any corrections to the low Mach number flamelet model. Berglund and Fureby [21] used a one-equation (mixture fraction) and a two-equation (mixture fraction and progress variable) flamelet model in conjunction with a two-step reaction mechanism. This combustion model is also based on the low Mach number flamelet approach without any compressibility correction. Vicquelin et al. [24] also developed a formalism to couple chemistry tabulation to solvers for mildly compressible flows. They computed temperature from the internal energy using a simple expansion, whereas no extension has been used for other quantities. This approach is reasonable for low Mach number compressible flows, but cannot accurately describe the high Mach number regime.

As shown in this study, the low Mach number assumption does not hold anymore at supersonic speed, where strong compressibility effects and viscous heating start to play an important role. For instance, the source term of the progress variable is extremely sensitive to the variations in temperature and pressure, and appropriate modifications should be implemented. Therefore, without appropriate compressibility corrections, a combustion model based on the low Mach number assumptions is not plausible for compressible flows, especially at high Mach numbers, where flows can admit shock waves and expansion fans.

We introduce here two different formulations of a compressible flamelet/ progress-variable approach, where temperature is not given by a chemistry table, but computed from the total energy and the species mass fractions. An analytical relationship is derived to eliminate costly iterative steps during the temperature calculation. In addition, the source term for the progress variable is rescaled by the mixture temperature and density, thus better accounting for compressibility effects on chemistry. Compressibility corrections have been devised also for the mixture properties, which are sensitive to the compressible variations of temperature and pressure. The model is tested in both LES and RANS computations for a reacting hydrogen jet in a supersonic transverse flow.

In the next section, the equations for the transported quantities are summarized. Section 3 describes the new combustion model and its implementation. The compressibility corrections are validated in Section 4 and applied to the case of a jet in a supersonic cross-flow in Section 5. The description of the flow configuration is given in Section 5.1, the numerical implementation in Section 5.2, and results are presented in Section 5.3. A sensitivity analysis of the proposed model to the model assumptions is provided in Section 6. Finally, we conclude with suggestions for future improvements.

2. Governing equations

In the following, we will discuss modeling of supersonic combustion both in the context of RANS and LES. The governing equations have a similar form, and, therefore, will be presented only once. The averaging operators appearing in these equations refer to an ensemble average in RANS, and to a spatial filter in LES. The relevant operators $\bar{\cdot}$ and $\tilde{\cdot}$ denote direct and Favre averaging or filtering, respectively.

Transport equations for the Favre averaged or filtered variables $\bar{\rho}$, $\bar{\rho}\tilde{u}_i$, $\bar{\rho}\tilde{E}$, $\bar{\rho}\tilde{Z}$, $\bar{\rho}\widetilde{Z''^2}$, and $\bar{\rho}\tilde{C}$ are solved in conservative form, where $\bar{\rho}$ is the density, $\tilde{u}_i$ the components of the velocity vector, $\tilde{E}$ the total energy, including the chemical energy, $\tilde{Z}$ the mixture fraction, $\widetilde{Z''^2}$ the variance of the mixture fraction, and $\tilde{C}$ a progress variable. Their respective transport equations are

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j}=0, \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial \bar{\tau}_{ji}}{\partial x_j}+\frac{\partial \bar{\tau}^R_{ji}}{\partial x_j}, \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t}+\frac{\partial \bar{\rho}\tilde{E}\tilde{u}_j}{\partial x_j}=-\frac{\partial \bar{p}\tilde{u}_j}{\partial x_j}+\frac{\partial \bar{\tau}_{ji}\tilde{u}_i}{\partial x_j}-\frac{\partial \bar{q}_j}{\partial x_j}+\frac{\partial \bar{\pi}^R_j}{\partial x_j}+\tilde{u}_i\frac{\partial \bar{\tau}^R_{ji}}{\partial x_j}, \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Z}}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}D_Z\frac{\partial \tilde{Z}}{\partial x_j}\right)+\frac{\partial \bar{\tau}^Z_j}{\partial x_j}, \tag{4}$$

$$\frac{\partial \bar{\rho}\widetilde{Z''^2}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\widetilde{Z''^2}}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}D_Z\frac{\partial \widetilde{Z''^2}}{\partial x_j}\right)+\frac{\partial \bar{\tau}^{Z''^2}_j}{\partial x_j}+2\frac{\mu_t}{\mathrm{Sc}_t}\frac{\partial \tilde{Z}}{\partial x_j}\frac{\partial \tilde{Z}}{\partial x_j}-\bar{\rho}\tilde{\chi}^R, \tag{5}$$

$$\frac{\partial \bar{\rho}\tilde{C}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{C}}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}D_C\frac{\partial \tilde{C}}{\partial x_j}\right)+\frac{\partial \bar{\tau}^C_j}{\partial x_j}+\bar{\dot{\omega}}_C, \tag{6}$$

where

$$\bar{\tau}^R_{ij}=\bar{\rho}\tilde{u}_i\tilde{u}_j-\bar{\rho}\widetilde{u_iu_j}, \tag{7}$$

$$q_i=-\frac{\lambda}{c_p}\frac{\partial h}{\partial x_i}+\sum_{\alpha=1}^{N}\left[\rho Y_\alpha V_{\alpha i}-\frac{\lambda}{c_p}\frac{\partial Y_\alpha}{\partial x_i}\right]h_\alpha, \tag{8}$$

$$\bar{\pi}^R_i=\bar{\rho}\tilde{e}\tilde{u}_j-\bar{\rho}\widetilde{eu_j}, \tag{9}$$

$$\bar{\tau}^Z_i=\bar{\rho}\tilde{u}_i\tilde{Z}-\bar{\rho}\widetilde{u_iZ}, \tag{10}$$

$$\bar{\tau}^{Z''^2}_i=\bar{\rho}\tilde{u}_i\widetilde{Z''^2}-\bar{\rho}\widetilde{u_iZ''^2}, \tag{11}$$

$$\bar{\tau}^C_i=\bar{\rho}\tilde{u}_i\tilde{C}-\bar{\rho}\widetilde{u_iC}, \tag{12}$$

μ and μ_t are the laminar and turbulent viscosity, k is the turbulent kinetic energy, λ the thermal diffusivity, c_p the specific heat capacity at constant pressure, Pr_t a turbulent Prandtl number, h the enthalpy including the sensible and chemical contributions, Y_k the species mass fractions, σ_k the turbulent kinetic energy Schmidt number,