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A robust numerical model for premixed flames with high density ratios based on new pressure correction and IMEX schemes

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ABSTRACT

In this study we present a model for the interaction of premixed flames with obstacles in a channel flow. Although the flow equations are solved with Direct Numerical Simulation using a low Mach number approximation, the resolution used in the computation is limited ($\sim$1 mm) hence the inner structure of the flame and the chemical scales are not solved. The species equations are substituted with a source term in the energy equation that simulates a one-step global reaction. A level set method is applied to track the position of the flame and its zero level is used to activate the source term in the energy equation only at the flame front. An immersed boundary method reproduces the geometry of the obstacles. The main contribution of the paper is represented by the proposed numerical approach: an IMEX (implicit–explicit) Runge–Kutta scheme is used for the time integration of the energy equation and a new pressure correction algorithm is introduced for the time integration of the momentum equations. The approach presented here allows to calculate flames which produce high density ratios between burnt and unburnt regions. The model is verified by simulating first simple solutions for one- and two-dimensional flames. At last, the experiments performed by Masri and Ibrahim with square and rectangular bodies are calculated.

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1. Introduction

Masri et al. [1], Ibrahim et al. [2,38] and Hargrave et al. [3] performed experiments with obstacles in a channel where a premixed flame was ignited. They found that the shape of the obstacles and their blockage ratio have influence on the flame speed and on the overpressure. The flame starts as a laminar front which generates a flow in the channel. Shear flow is produced by the obstacles and the level of turbulence starts to rise. As a consequence the flame is wrinkled and its surface area increases. The propagation speed is proportional to the flame surface and increases. It is clear that the possibility to predict such interaction can help to improve the design of complex systems like for instance, industrial plants and to reduce the risk in case of deflagrations.

The aim of this work is mostly numerical with the scope of proposing a stable algorithm for high density ratio flames like in the case of Masri et al. experiments. Simplifications are adopted to overcome the limitations represented by the complex chemical mechanisms of the premixed combustion process. The proposed model is able to avoid the numerical instabilities that could arise during the computation of premixed flames with high density rations and heat transfer with obstacles. Our computations use DNS (Direct Numerical Simulation) for the resolution of the flow equations although due to the low resolution adopted ($\sim$1 mm) the smallest flame/vortex interactions will probably not be captured. While the inner structure of

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the flame and the chemical scales are not solved, the reacting part (energy equation with source term) is modeled with a level set approach (G-equation, [4]). This approach removes the need for solving the detailed chemistry and does not require a model for the turbulence. The G-equation does not interact directly with the flow, it simply tracks the position of the flame and its zero level location is used to activate the source term in the energy equation at that location where the flame front is located for each particular time.

This work is organized in three main sections. In the first section the governing equations are introduced, in the second one the numerical methods for their integration are presented together with a stability analysis. In the third section results for simple cases and for the interaction of a premixed flame with obstacles are presented and discussed. In particular, we reproduce the experiment performed by Ibrahim [2,38] in which the speed of the flame front was measured.

1.1. The set of equations

A system of equations that allows for large heat release, large temperature and density variations and substantial interaction with the hydrodynamic flow field including the effects of the turbulence is required. A low Mach number approximation is suitable in such a case with remarkable advantages regarding the implementation because we do not have to resolve the acoustic oscillations and the set of equations is similar to the incompressible case but the density may vary due to heat release [5–7].

Following the asymptotic derivation given by Buckmaster and Ludford [41] or recently found also in Müller [8], it can be shown [33] that the non-dimensional set of continuity, momentum and temperature equations (with source term $\dot{\omega}$) in low Mach number approximation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \frac{1}{Re} \nabla \cdot \tau \tag{2}$$

$$\rho \frac{\partial T}{\partial t} + \rho u \nabla \cdot T = \frac{1}{Re\,Pr} \nabla \cdot (\lambda \nabla T) + \rho \dot{\omega} \tag{3}$$

With ρ being the density, u the velocity, p the dynamic pressure, T the temperature, λ the thermal conductivity (taken here constant and scaled such that it is equal to unity) and τ the Newtonian stress tensor. An equation of state for ideal gas is also used,

$$p_0 = \rho T \tag{4}$$

In this derivation the thermodynamic pressure p_0 has been assumed constant and the influence of gravity is neglected. Moreover the effect of viscous dissipation in the energy equation drops out as a result of the approximation.

The position of the flame is found by solving a level set equation whose variable G is defined as a distance function [4]. The G-equation describes the evolution of the front as a level set function that is continuous through the flame front [44]. An implicit representation of the instantaneous flame surface can be given as [44]

$$G(x_f, t) - G_0 = 0 \tag{5}$$

which defines the level set function G. Here, t is the time and x_f is the vector of the flame front location. Differentiating the previous equation with respect to time one obtains

$$\frac{\partial G}{\partial t} + \frac{dx_f}{dt} \cdot \nabla G = 0 \tag{6}$$

The flame front propagation speed is given by

$$\frac{dx_f}{dt} = u + s_l n \tag{7}$$

where u is the local flow velocity, s_l is the laminar burning speed and n is the flame normal defined to be directed into the unburned mixture and its expression is

$$n = -\frac{\nabla G}{|\nabla G|} \tag{8}$$

By imposing $|\nabla G| = 1$ (everywhere in the domain by a reinitialization procedure) this makes sure that the G values give always the distance form the zero level. The advantage of G being a distance function is that it is now not necessary to track the position of the flame front in order to determine the distance from the flame front at a certain point x since this distance now is given by $G(x) - G_0$ and if G_0 is assumed as origin of the coordinates then it is given by $G(x)$.

The laminar burning speed, s_l may be different from the unstrained laminar burning speed (let us call it s_L^0) because of the shape of the flame that changes during the propagation forming points where the speed is higher than s_L^0 due to the effect of the flame stretch.

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