Combustion and Flame 163 (2016) 508–516

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

A diffuse interface method for simulating the dynamics of premixed flames

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ARTICLE INFO

Article history:
Received 1 July 2015
Revised 20 October 2015
Accepted 20 October 2015
Available online 27 November 2015

Keywords:
Premixed flames
Numerical simulation
Diffuse interface
Lattice Boltzmann method

ABSTRACT

A diffuse interface method for simulating dynamics of premixed flames is proposed. The flame is treated as a diffuse moving front with its propagation automatically captured by the convection–diffusion equation of the progress variable. The diffusion and reaction terms are constructed using the flame speed and flame thickness, and the flame speed is taken as a function of the local stretch rate to incorporate the stretch effect. This equation is coupled with the continuity equation and the momentum equation to describe flame dynamics in complex flows, and the lattice Boltzmann method is employed in the present study as the computational platform, since its feature of explicit computation is highly consistent with the advantage of flame auto-capturing of the present method. To test the performance of the method, simulations including 1-D flame propagation, 2-D Darrieus–Landau instability, 2-D cylindrical flame propagation with stretch effect, and 2D flame–vortex interaction are conducted, and the consequent results are in good agreement with analytical solutions.

1. Introduction

While the numerical simulation of reacting flows can be exceedingly challenging and time-consuming due to the strong non-linearity of the flow as well as the non-linearity and stiffness of the chemical kinetics [1], several methods have been developed [2–5] for the dynamics of premixed flames by treating the flames as moving fronts. Prominent among them is the level set or the G-equation method, in which the flame is assumed to be infinitely thin and thereby represented by an iso-surface of the level set function G. The local propagation speed of the flame surface, $\boldsymbol{V}_f = d\boldsymbol{x}/dt|_{G=G0}$, is directly specified to be $\boldsymbol{V}_f = \boldsymbol{v}|_{G=G0-} + s_u\boldsymbol{n}$, where $\boldsymbol{v}|_{G=G0-}$ is the local flow velocity on the unburnt side and $\boldsymbol{n}$ the unit normal vector, such that the flame propagates towards the unburnt mixture at the given flame speed s_u [2,3]. However, since the flame is assumed to be infinitely thin, no information on the thermal structure is provided. As a result, it is intrinsically inadequate to describe problems in which the flame thickness is comparable to the length scale of the phenomenon being examined, *e.g.* flame–flame or flame–vorticity interactions. Furthermore, in order to yield robust numerical results, the level set function has to be re-initialized frequently during the evolution in order for it to remain a signed distance function, which renders the computation rather complicated and may even bring about additional numerical error.

Recognizing that fluid mechanically premixed flames share much similarity with two-phase flows, in that the density jumps across an interface but remains incompressible in the bulk phases (only low Mach number flow is considered), it is conceptually expected that the numerical methods for them should be analogous, even though the interfaces are characterized by flame propagation and surface tension respectively. Consequently the level set and front-tracking methods for premixed flames have been widely used in two-phase flow problems without significant modification [6–10].

In recent years, the diffuse interface method, also known as the phase-field method, has proven to be successful in modeling two-phase flows including phase transition [11,12], droplet/bubble dynamics [13–15], as well as moving contact line motion [16,17]. In this method, the fluid composition is represented by an order parameter that remains constant in the bulk phases while varies rapidly but smoothly across the interface, resulting in a finite thickness structure rather than a discontinuity description of the interface. Besides, the order parameter is able to self-sustain its equilibrium profile by minimizing the total free energy without additional treatment, *i.e.* the interface can be captured automatically. Compared to the level set method and the front tracking method, the diffuse interface method is physically clearer and numerically much simpler, which makes it particularly efficient when dealing with complicated topological

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http://dx.doi.org/10.1016/j.combustflame.2015.10.027
0010-2180/

changes. It is therefore of interest if the similar methodology can be adopted for premixed flames. In this regard we note that Khokhlov [18] proposed a flame-capturing technique (FCT) to simulate flames in astrophysical applications. Instead of being treated as discontinuities, flames in FCT are diffused over several grids and captured by an advection–diffusion-reaction (ADR)-type equation. However, due to the insignificant density jump across astrophysical flames (only about 10%), thermal expansion effect was not considered in the model. Vladimirova et al. [19] and Zhiglo [20] further included density variation in the flame capturing equation for simulating terrestrial flames with large density jumps. To get the correct flame speed, Vladimirova et al. [19] used a calibration factor to the mapping of flame speed and flame thickness to the diffusion and reaction terms respectively, while the calibration factor would depend on the specific type of reaction rate; Zhiglo [20] analytically derived the flame speed and flame thickness for constant diffusivity and step-function/KPP reaction rates, with both the flame speed and flame thickness being dependent on the thermal expansion ratio. Furthermore, although the flame thickness could be kept finite by taking the diffusivity as a function of the progress variable, fitting is still inevitable in determining the flame speed from the diffusion and reaction terms.

It is also recognized that numerically solving the moving front/interface together with the Navier–Stokes equations could be rather complicated since the moving front/interface equation, continuity equation, and momentum equation are strongly coupled. However, from a mesoscopic point of view, the fluids can be treated as discrete particles whose evolution is governed by the Boltzmann equation, and the macroscopic variables such as density, momentum and pressure can be readily obtained by taking moments of the distribution function. As a numerical tool to solve the Boltzmann equation, the lattice Boltzmann method (LBM) discretizes the continuous particle velocity space into a finite set of fixed velocities, such that the convection term becomes linear and the calculation is greatly simplified into the explicit "collision–streaming" scheme. Due to the remarkable convenience in numerical implementation, the flexibility in handling complex boundary and the efficiency in parallel computation, LBM has gained increasing popularity as a promising alternative CFD technique [21]. Specifically, in the field of combustion research, LBM has been employed as an efficient flow solver to simulate reactive Rayleigh–Taylor systems [22], premixed flames [23–26] and diffusion flames [27], although modeling premixed flames as moving fronts has not been implemented.

In the present study, we propose a diffuse interface method to simulate the dynamics of premixed flames. In the framework of the FCT-ADR approach, a new flame capturing equation is developed with the diffusion and reaction terms constructed using the flame speed and thickness, and the thermal expansion as well as stretch effects are taken into account. It is noted that although the present method can be numerically solved through various ways without difficulty, LBM is employed as the computational platform since its feature of explicit computation is highly consistent with the advantage of interface auto-capturing of the present method.

In the following the methodology, numerical examples and conclusions are sequentially presented, in Sections 2 through 4.

2. Methodology

2.1. Macroscopic governing equations

To model premixed flames as moving fronts, the unburnt mixture, burnt mixture, as well as the flame front should be first characterized. It is noted that in two-phase flows, a field variable, named composition and stands for the volume fraction of one fluid, is usually employed to distinguish the computational domain into different phases [13–15]. For premixed flames, a similar and appropriate choice is the progress variable C defined by

$$C = \frac{T - T_u}{T_b - T_u} = \begin{cases} 0, & \textit{unburnt mixture} \\ 0 \sim 1, & \textit{flame front} \\ 1, & \textit{burnt mixture} \end{cases}, \tag{1}$$

where T is the local temperature, and the subscripts u and b denote unburnt and burnt mixtures respectively. Realizing that flame propagation is driven by diffusion and reaction, the evolution of C is described by the convection–diffusion equation [19,20]:

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial(\rho C u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho D \frac{\partial C}{\partial x_j}\right] + \dot{\omega}, \tag{2}$$

in which ρ is the density, u the velocity, D the diffusivity of C, and $\dot{\omega}$ the chemical source term. From scaling analysis, since ρD and $\dot{\omega}$ are correlated with the flame speed s_u and the flame thickness δ through $\rho D \sim \rho_u s_u \delta$ and $\dot{\omega} \sim \rho_u s_u/\delta$, they can respectively assume the forms:

$$\rho D = \alpha \rho_u s_u \delta \tag{3}$$

and

$$\dot{\omega} = \frac{\rho_u s_u}{\delta}\Omega(C), \tag{4}$$

where α is a positive constant and $\Omega(C)$ a function of C. Then, by substituting Eqs. (3) and (4) into Eq. (2), the transport equation for C becomes:

$$\frac{\partial(\rho C)}{\partial t} + \frac{\partial(\rho C u_j)}{\partial x_j} = \alpha \rho_u s_u \delta \frac{\partial^2 C}{\partial {x_j}^2} + \frac{\rho_u s_u}{\delta}\Omega(C) \tag{5}$$

such that the remaining problem is to determine the expression for $\Omega(C)$.

For 1D planar flame propagation (in the x direction), when the inflow velocity from the unburnt mixture equals to the flame speed s_u, the flame would remain stationary, *i.e.* $\partial/\partial t = 0$, and $\rho u \equiv \rho_u s_u$ is valid throughout the flow. In this case, Eq. (5) is simplified to:

$$\frac{\partial C}{\partial x} = \alpha\delta\frac{\partial^2 C}{\partial x^2} + \frac{1}{\delta}\Omega(C). \tag{6}$$

Considering that C ranges from 0 to 1 and the flame has a finite thickness of δ, it is reasonable that C assumes the profile

$$C(x - x_0) = \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{x - x_0}{\delta}\right), \tag{7}$$

where x_0 is the location of $C = 0.5$. It is noted that this profile agrees well with the real structure of premixed flames [1] and has been also used to describe the diffuse interface in two-phase flows [13–15]. Then, by substituting Eq. (7) into Eq. (6) and noting that $d(\tanh\Phi)/d\Phi = 1 - 2\tanh^2\Phi$, the expression for $\Omega(C)$ is obtained as:

$$\Omega(C) = 2C(1 - C)[4\alpha C - (2\alpha - 1)]. \tag{8}$$

By further substituting the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \tag{9}$$

into the left hand side of Eq. (5), the transport equation for C then becomes:

$$\rho\left(\frac{\partial C}{\partial t} + u_j\frac{\partial C}{\partial x_j}\right) = \alpha\rho_u s_u\delta\frac{\partial^2 C}{\partial {x_j}^2} + \frac{2\rho_u s_u}{\delta}C(1 - C)[4\alpha C - (2\alpha - 1)]. \tag{10}$$

As mentioned above, α is defined as a positive constant in the diffusion term. Since it is now also included in the reaction term, its range should be determined more rigorously to ensure numerical robustness. To do this, the homogenous mixture without diffusion is considered. In this case, the mixture has two stable states, namely the