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A front propagation formulation for under-resolved reaction fronts

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ABSTRACT

A method to simulate propagating reaction fronts on under-resolved grids is presented. The proposed method prevents the spurious propagation of under-resolved reaction fronts by introducing a front propagation form of the chemical reaction term. The front propagation formulation adopts a regularized Delta function to discretely preserve the total reaction rates on computational grids. By introducing the regularized Delta function that reproduces the physical mechanism of front propagation, the present method allows for the simulation of reaction fronts with variable thicknesses on under-resolved grids. Applications to isothermal reaction fronts, laminar premixed flames, and large eddy simulation of turbulent premixed flames are presented.

1. Introduction

Propagating reaction fronts are widely observed in engineering applications and nature. In many cases, the propagation of the reaction fronts is governed by the balance of diffusion and reactions, and such fronts are convected and stirred by fluid flow. The correct prediction of the propagation speed requires that the reaction–diffusion balance in the reaction fronts is well described. When the thickness of a reaction front is of the order of the smallest flow length scale or even thinner, accurate prediction of front propagation requires much higher spatial grid resolution than that normally used for fluid flow. The computational cost of simulating front propagation then increases significantly. The focus of this paper is on the simulation of such reaction fronts on under-resolved grids. Here, the term “under-resolved” is used to indicate that the grid resolution is not fine enough to capture the inner structure of propagating reaction fronts.

A traditional solution for this problem is to track a reaction front. In the level set method [1–4], for instance, the movement of a reaction front is tracked in an Eulerian manner by solving the level set equation on a regular grid. The reaction fronts are represented by isosurfaces of the so-called level set function G. The value of G is defined to be G_0 at sharp reaction fronts, and the propagation speed of the iso-G_0 surfaces is prescribed. The G fields other than the front surfaces are arbitrary and typically defined as smoothly varying function, e.g., a signed distance function. By ‘tracking’, and not ‘resolving’, a reaction front, the level set method does not suffer from the resolution requirement for the reaction–transport balance in the thin fronts. While the level set method is widely used in simulations of sharp interfaces in multiphase flows [5,3], the application and the formulation for propagating reaction fronts, in particular premixed flames, have been reported in [2,4,6–14], among others.

In this paper, a new method to simulate propagating reaction fronts on under-resolved grids, called the front propagation formulation (FPF), is proposed. A distinct feature of the proposed method is that it can be applied not only to sharp

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fronts but also to reaction fronts with variable thicknesses. The main idea is to adopt a regularized Delta function to preserve the local propagation characteristics of a reaction front regardless of resolution levels. The regularized Delta function that is based on the physics of the reaction–transport balance in propagating fronts, thereby allowing for simulations of variable-thickness reaction fronts, is proposed. In what follows, the model formulation is presented. The regularized Delta function that preserves the reactive nature of propagating fronts is presented, and the relationship of the regularized Delta function to chemical reaction rate terms is discussed. A method to incorporate a curvature-dependent propagation speed is described. Applications to isothermal reaction fronts, laminar premixed flames, and large eddy simulation (LES) of turbulent premixed flames are then presented.

2. Model formulation

2.1. Front propagation formulation for chemical reaction terms

A key physical quantity to describe propagating reaction fronts is the progress variable c, which represents the progress of reactions from the unreacted ($c = 0$) to the fully reacted side ($c = 1$). The equation for the progress variable can be written as

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho \mathbf{v} c) = \nabla \cdot (\rho D \nabla c) + \rho \omega_c, \tag{1}$$

where ρ is the density, $\mathbf{v}$ is the fluid velocity, D is the molecular diffusion coefficient, and ω_c is the chemical reaction source term. Fick's law of diffusion is assumed.

The front propagation is typically characterized by the propagation speed of the front. The consumption speed of the front can be defined as

$$s_c = \frac{1}{\rho_u} \int_{n_0}^{n_1} \rho \omega_c \lambda dn, \tag{2}$$

where s_c is the consumption speed and ρ_u is the density of an unreacted mixture. The front normal vector is defined as $\mathbf{n} = \nabla c / |\nabla c|$, and n is the coordinate in the front normal direction. The reaction rates along the front normal coordinate are significant only between n_0 and n_1. For a steady 1-D planar front, by integrating Eq. (1) from the unreacted side to the fully reacted side, it can be shown that Eq. (2) with $\lambda = 1$ represents the propagation speed of a steady planar front. A geometric factor λ is introduced to preserve overall consumption of an unreacted mixture for multi-dimensional problems. Note that in the proposed method, this equation 'formally' defines the propagation speed. When applied to actual simulations, the propagation speed is specified and plays essentially the same role as the speed of the G_0 surface in the level set method. The explicit expression of the λ factor is necessary only when evaluating the consumption speed from fully resolved simulations or experiments. More details of the geometric factor λ can be found in Bell et al. [15], for example. In highly under-resolved reaction fronts, the reaction rates represented by the grid points along the front normal direction, $\mathbf{n}$, are very different from the actual values. For these under-resolved fronts, the integrated reaction rates or the consumption speed can be quite erroneous. Under such conditions, the overall front propagation cannot be predicted with accuracy.

Here, a new reaction rate formulation that discretely preserves the overall reaction rates on a computational grid and hence the front propagation characteristics regardless of resolution levels is presented. The total reaction rates in the domain Ω can be written as

$$S_{T,\Omega} = \int_{\Omega} \rho \omega_c d\mathbf{x} = \int_{A_s} \rho_u s_c dA = \int_{\Omega} \rho_u s_c \delta\big(\mathbf{n} \cdot (\mathbf{x} - \mathbf{x}_s)\big) d\mathbf{x}, \tag{3}$$

where Ω is large enough to contain reaction fronts. A_s is a surface that propagates with the consumption speed s_c, and $\mathbf{x}_s$ is the location of that surface. In Eq. (3), the consumption speed is implicitly defined to represent the propagation speed of 'a front surface'. δ is the Dirac delta function. In numerical computation, the Dirac delta function δ is approximated using the regularized Delta function δ_Δ, where Δ represents the scale of grid spacing. The reaction rates can then be written as

$$\rho \omega_c = \Psi = \rho_u s_c \delta_\Delta \big[\mathbf{n} \cdot (\mathbf{x} - \mathbf{x}_s)\big]. \tag{4}$$

The form Ψ is called the front propagation form of chemical reaction rates here. In FPF, the integrated reaction rates are redistributed in the proximity of the front surface A_s in such a way that the total reaction rates in Eq. (3) are invariant of resolution levels. This type of approach is commonly used in the computation of multiphase flows, e.g., the continuum surface force method [16]. The existing formulations for the regularized Delta function are, however, not designed to reproduce the characteristics of the reaction front.

2.1.1. Front structure function

The primary feature of the proposed formulation is the preservation of the local propagation characteristics of a reaction front regardless of resolution levels. This is achieved by distributing the integrated reaction rates (consumption speed) over