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A dynamic model for the turbulent burning velocity for large eddy simulation of premixed combustion

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Abstract

Turbulent premixed combustion is particularly difficult to describe using large eddy simulation (LES). In LES, premixed flame structures typically exist on subfilter length scales. Consequently, premixed LES models must be capable of describing how completely unresolved flame structures propagate under the influence of completely unresolved eddies. This description is usually accomplished through the implementation of a model for the turbulent burning velocity. Here, a dynamic model for describing the turbulent burning velocity in the context of LES is presented. This model uses a new surface filtering procedure that is consistent with standard LES filtering. Additionally, it only uses information that comes directly from the flame front. This latter attribute is important for two reasons. First, it guarantees that the model can be consistently applied when level set methods, where arbitrary constraints can be imposed on field variables away from fronts, are used to track the flame. Second, it forces the model to recognize that the physics governing flame front propagation are only valid locally at the front. Results showing model validation in the context of direct numerical simulation (DNS), and model application in the context of LES, are presented.
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Keywords: Premixed turbulent combustion; Burning velocity; Large eddy simulation; Level set methods; Dynamic model

1. Introduction

Turbulent premixed flames are particularly difficult to describe in the context of large eddy simulation (LES). Most industrially relevant premixed flames exist in either the corrugated flamelets regime or the thin reactions zones regime [1]. The width of the inner reaction zone of a flame in these regimes is comparable to, if not smaller than, the Kolmogorov length scale that describes the size of the smallest turbulent eddies in the flow. Flame preheat zones, which are typically much broader than reaction zones, may also, in the corrugated flamelets regime, exist on sub-Kolmogorov length scales. In LES, by definition, the smallest length scales of a flow are filtered out. As a result, in industrially relevant regimes the transitions that occur between unburned and burned states occur mostly on subfilter scales.

Premixed combustion models for implicitly filtered LES that use standalone progress variable or finite rate chemistry approaches will thus, it seems, always fail. All models are limited by the accuracy of the schemes they use for evaluating gradients, and no scheme is capable of resolving the sharp subgrid transitions that occur in premixed implicit LES near flame

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fronts. Premixed implicit LES models that attempt to resolve flame structure are therefore especially prone to numerical errors in the most critical regions of the flowfield.

A variety of methods have been suggested in the literature in response to the problem of subgrid transition. Two of the most widely discussed are level set, or G-equation, methods, and artificial flame thickening methods. The dynamically thickened flame model, for example, uses finite rate chemistry, but additionally broadens local reaction zones so that they can be resolved on LES meshes [2]. This broadening is achieved by increasing molecular diffusivities and, in a proportionate manner so as to keep the laminar flame speed constant, spreading out the influence of reaction source terms. Thickened flame models therefore eliminate the problem of poor resolution. The thickening procedure, however, has an important consequence. The widened flame attenuates local turbulence and prevents eddies smaller than the thickening length scale from influencing the front. This effectively decreases the velocity at which the front propagates and creates the need for a compensating model. The so-called "efficiency function" that is used acts to ensure that the flame will propagate at appropriately large speeds in the presence of turbulence [3]. This efficiency function may in one sense be viewed as the empirical introduction of a model describing the turbulent burning velocity.

In level set methods, flame fronts are characterized using isocontours of field variables and explicitly tracked [1,4–7]. At the relevant isocontours, the field variables are governed by equations describing how the fronts propagate. Away from the relevant isocontours, smooth gradients are prescribed for the field variables to ensure numerical resolution of front dynamics. In level set methods, the inner reaction zones of premixed flames are treated as coherent structures. The effect of the chemical activity that occurs within these reaction zones appears in the governing front equation almost entirely as a front propagation speed. This speed is approximately equivalent to the laminar burning velocity in the fully resolved case. Due to the coherent treatment of inner reaction zones, level set approaches suffer from the drawback of not being able to inherently consider local flame quenching. Conversely, they offer the advantage of not inducing any artificial interactions between the heat released by the flame and the flow field. Both the laminar unstretched burning speed and its dependence on the local flame stretch rate appear as external parameters in level set methods. These parameters are typically well described by both experiments and computational chemical kinetics studies, and can be used with confidence in simulations. When level sets are used in the context of LES, however, filtered descriptions of the burning velocity that account for subfilter turbulence are additionally needed.

In non-premixed combustion, the great advantage that LES offers is that the scalar mixing process is reasonably resolved [8,9]. In premixed combustion, the scalar mixing process is also important, but it remains poorly resolved at the flame front in most LES situations. The turbulent burning velocity, which is needed in both of the premixed modeling approaches discussed here, is a quantity that expresses how this unresolved mixing process interacts with chemistry. Traditional burning velocity models rely on a series of coefficients that have been determined through analyses of both experimental and direct numerical simulation (DNS) data [6,10]. These coefficient-based approaches have been successfully applied in Reynolds averaged Navier–Stokes (RANS) simulations, where level set methods offer an alternative to the problem of reaction rate closure [6,11]. In LES, however, where instantaneous flame realizations are available, it is possible to eliminate the use of constant coefficients by employing dynamic procedures to determine coefficients automatically.

The general dynamic procedure has been employed by a variety of researchers in their efforts to deal with closure problems in reacting flows. Direct reaction rate closure is a particularly challenging problem because reaction rates strongly depend on the exact flow and chemical conditions that are present on the smallest turbulent scales. Dynamic procedures have therefore been applied to combustion models that use indirect techniques to account for reaction rates. Two such approaches are the previously discussed thickened flame model, and flamelet-type models, where it is assumed that small scale flame structures can be precomputed as a function of turbulent parameters. Charlette et al. [12,13], for example, use a dynamic approach to determine a parameter in the "wrinkling factor" that appears in the thickened flame model. Knikker et al. [14] dynamically determine a parameter for this same wrinkling factor but apply it in the context of the flame surface density model. Chakraborty and Cant [15] developed a method of dynamically determining the surface averaged curvature that appears in the flame surface density model.

Additionally, dynamic procedures have been applied in the context of level set modeling. Im et al. [16] and Bourlioux et al. [17], for example, proposed a dynamic propagation model that treats level set field variables as scalars. Subfilter contributions to flame propagation speed are determined by evaluating a burning velocity model at two different filter levels and comparing the results to differences in the magnitude of the gradient of the level set field variable at those same two levels. Im et al. [16] claim that this

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