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Role of the progress variable in models for partially premixed turbulent combustion

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Abstract

It is shown that if partially premixed combustion is described in terms of a mixture fraction and a progress variable, scalar dissipation terms appear in the transport equation for the progress variable. These terms are essential if not only the fully premixed limit but also the transport equation for a classical diffusion flame are to be recovered. The eddy breakup relationship between mean rate of reaction and scalar dissipation is extended to partially premixed combustion at high Damköhler numbers. Advantages and disadvantages of working in terms of a progress variable rather than a major species mass fraction or temperature are identified and discussed.

Keywords: Turbulent combustion; Partial premixing; Progress variable

1. Introduction

Many theoretical models of turbulent combustion processes assume either that fuel and oxidiser are fully premixed prior to combustion or that they enter the flame zone separately. However, in reality, this is often not the case. The burning of, for example, liquid fuel sprays can involve an intermediate regime in which the fuel and oxidiser are partially mixed at the time of combustion [1], and many practical combustion devices, including reciprocating engines, gas turbines, and furnaces, often operate in a partially premixed burning regime. Modern combustion practice involves careful control of the extent of partial premixing in order to minimise pollutant emissions while avoiding undesirable combustion instabilities.

In most practical systems, stable and efficient burning is obtained when chemical time scales are short in comparison with fluid mechanical time scales, that is, at large Damköhler numbers. As a consequence, combustion frequently occurs in a "thin flamelets" or "thin reaction zones" burning regime, in which chemical reaction is confined to narrow regions or flamelets, whose structure may or may not resemble that of a laminar flame and whose thickness is small compared to some or all of the characteristic scales of the flow. The archetypical laminar partially premixed flame is the triple flame or edge flame, consisting [2] of fuel-rich and fuel-lean premixed flame branches joined at the triple point to a trailing diffusion flame. Thin fuel-rich and fuel-lean premixed flamelet regions may be expected, which can be iden-

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tified from the criterion [3] $\nabla Y_F \cdot \nabla Y_{Ox} > 0$, where the reacting mixture is described in terms of the fuel, oxidiser, and product mass fractions, Y_F, Y_{Ox}, and Y_P, respectively, and there are also thin diffusion flamelet regions for which $\nabla Y_F \cdot \nabla Y_{Ox} < 0$; the three types of flamelets meet at triple points.

Two different types of partially premixed burning may be distinguished: if only fuel-rich or only fuel-lean mixture can exist, then diffusion flames will not occur. This is sometimes referred to as "stratified premixed combustion." The present paper is primarily concerned with the more general situation, which can occur in spray combustion, for example, where the existence of both fuel-rich and fuel-lean pockets may lead to a combination of premixed and diffusion flame burning. In many combustion systems, flame stabilisation is achieved after the recirculation of burnt gases, and partial premixing with hot products may also be observed. A generic configuration for fundamental studies of partially premixed gaseous combustion and for the development of theoretical models is the lifted turbulent flame, which is observed when a fuel jet emerges into oxidiser at too high a velocity for a flame to stabilise at the fuel nozzle exit [4–9]. When some vitiated gases are added at injection, as in the experiment in [10], the partial premixing with burnt gases is also addressed.

Existing theoretical models of turbulent combustion can be divided into various categories [11–13]. At first sight, transported pdf models [14] appear to be widely applicable, independently of the degree of premixing between fuel and oxidiser, because the chemical source term in the pdf transport equation is closed, and so requires no modelling. However, the so-called mixing term, which can be related to the scalar dissipation, is unclosed. Models for this term are often based on an assumption that mixing is due to turbulence and is not directly linked to chemical reaction [14], but this assumption cannot be valid in the laminar flamelet combustion regime. For premixed combustion in this regime, it was shown in [15] that the mixing term can be successfully represented as the sum of a term depending on laminar premixed flame properties and a second term containing turbulence parameters. An extension of this concept to partial premixing might lead to a mixing model in terms of properties of both laminar premixed flames and laminar diffusion flames, as well as turbulence parameters. It is not clear how such a model could be constructed.

A second and simpler category is the presumed pdf model. In applications to partially premixed combustion [16,17], the form of the joint pdf of two composition variables, typically a mixture fraction and a major species mass fraction or progress variable, is represented empirically and controlled by first and second moments of the two scalar variables, which are obtained from modelled transport equations. Problems here include the shape of the presumed joint pdf—can the two scalar variables be assumed to be statistically independent?—and appropriate models for the various scalar dissipations appearing in the second moment equations. At high Damköhler numbers, these models lead to simple relationships between mean reaction rate and scalar dissipation, both for fully premixed burning [18] and for combustion in diffusion flames [19]. An equivalent relationship for partially premixed combustion is developed in the present work.

Thin flamelet models for partially premixed combustion are sometimes based on the level-set formulation of Peters [11] or on the concept of a flame surface density, or flame surface area per unit volume, as in the coherent flame model [20]. In both cases, and also in some presumed pdf models, premixed and diffusion flame models are introduced separately, and assumptions must be made in order to determine the proportion of each burning mode at every location in the flame [21]. A recent example of a calculation making use of separate laminar flamelet models for local premixed and diffusion flame burning in partially premixed combustion is provided by the large eddy simulation reported in [8,9], where a flame index, which takes a value of unity in a premixed flamelet and zero in a diffusion flamelet, is modelled and used to determine the proportions of premixed and diffusion flamelet burning in each computational cell of the LES. Two important scalar variables in the analysis are a mixture fraction and a progress variable, which is defined in terms of a normalised fuel mass fraction. In the partially premixed case, the normalisation process is shown to introduce a dependence on the mixture fraction, and this leads to the appearance of two scalar dissipation terms in the transport equation for the progress variable. Similar observations, restricted to fuel-lean mixtures, have been made by others [22,23]. In the special circumstances of this LES [8], where the flame index ensures that either a premixed or a diffusion flamelet is to be represented, it is argued that the additional terms can be neglected. However, this needs not always be the case.

The progress variable, which is familiar in premixed combustion studies [24], has also been used in RANS models of partially premixed turbulent combustion [25], with a modelling formalism organised in such a way that the additional terms found in [8] are avoided. On the other hand, the additional terms were neglected in a transported pdf study [26] of turbulent autoignition in terms of mixture fraction and progress variable. Those terms were also absent in recent LES of nonpremixed flames that use a diffusion flamelet approach combined with a progress variable [27]. The aims of the present work are to ex-