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Scalar dissipation and mean reaction rates in premixed turbulent combustion

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ABSTRACT

A general equation for a variance parameter, appearing as a crucial quantity in a simple algebraic expression for the mean chemical rate, is derived. This derivation is based on a flamelet approach to model a turbulent premixed flame, for high but finite values of the Damköhler number. Application of this equation to the case of a planar turbulent flame normal to the oncoming flow of reactants gives good agreement with DNS data corresponding to three different values of the Damköhler number and two values of the heat release parameter.

1. Introduction

Premixed turbulent combustion can be described in terms of a combustion progress variable $c(x,t)$, with $c = 0$ in reactants and $c = 1$ in products, satisfying the equation

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

where ρ, $\mathbf{u}$ and D represent gas density, flow velocity and diffusion coefficient, respectively, and ω_c is the chemical reaction rate [1]. Prediction of its mean value $\bar{\omega}_c$ either in RANS or LES calculations is one of the most difficult problems in turbulent combustion modelling [2,3]. One way to address this problem is through a presumed pdf model in which the mass-weighted pdf $\tilde{P}(c;\ \mathbf{x},\ t)$ is assumed to have a specified shape controlled by the first and second Favre moments of c, so that $\tilde{P}(c;\ \mathbf{x},\ t) = \tilde{P}(c;\ \tilde{c}(\mathbf{x},\ t),\ \widetilde{c''^2}(\mathbf{x},\ t))$.

An analysis of three different presumed pdf models [4] at large values of the Damköhler number $Da = t_t/t_c$, where t_t and t_c are characteristic turbulence and chemical time scales, leads to the simple result that

$$\bar{\omega}_c = \epsilon_{cc} B \bar{\rho} \tilde{c}(1-\tilde{c}) I \tag{2}$$

where B, in s^{-1}, is the constant coefficient of the pre-exponential factor in the global reaction rate expression, and I is an integral quantity defined later on (see Eq. (38)), whose value depends on the reaction rate expression as well as the shape of the selected pdf [4]. Although I is known for a given pdf, its value is uncertain to the extent that the shape of the pdf is an approximation. Also ϵ_{cc} is related to the variance $\widetilde{c''^2}$ by

$$\epsilon_{cc} = 1 - \frac{\widetilde{c''^2}}{\tilde{c}(1-\tilde{c})} \tag{3}$$

so that ϵ_{cc} is equal to unity if $\widetilde{c''^2} = 0$ and is zero if $\widetilde{c''^2}$ reaches its maximum possible value of $\tilde{c}(1-\tilde{c})$. In the latter case, for which $Da \gg 1$, $\tilde{P}(c;\mathbf{x},t)$ is bimodal and consists only of delta functions at $c = 0$ and $c = 1$. Before Eq. (2) can be used it is necessary to derive either an expression for ϵ_{cc} or a balance equation for this quantity.

The Favre mean $\tilde{c}(\mathbf{x},t)$ and variance $\widetilde{c''^2}(\mathbf{x},t)$, which determine the shape of the presumed pdf $\tilde{P}(c;\mathbf{x},t)$, must be calculated from closed transport equations. To do so, in addition to several other closure problems, a model must be provided for the mean scalar dissipation which appears as a sink term in the variance equation. The mean scalar dissipation is a measure of the rate at which molecular diffusion processes lead to small-scale mixing in turbulent flows. It plays an important role in many theoretical descriptions [5–9] of the mean rate of chemical reaction in turbulent combustion, particularly when $Da \gg 1$. If the fuel and oxidiser are supplied to the combustion zone separately, the scalar dissipation describes the rate at which they mix and burn. In the case of premixed combustion the scalar dissipation represents the rate at which cold unburned reactants and hot fully burned products are mixed and burned. It is defined as

$$\tilde{\chi} = \overline{\rho D \nabla c'' \cdot \nabla c''}/\bar{\rho} \tag{4}$$

If $Da \gg 1$, combustion is confined to thin propagating reaction zones, whose internal structure resembles that of a laminar flame, and which separate unburned reactants from combustion products. The composition gradient appearing in Eq. (4) is then related to that in a laminar flame. Theory [10,11] and DNS [12] both show that if $Da \gg 1$ the scalar dissipation $\tilde{\chi}$ is proportional to the chemical

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source term $\bar{\omega}_c$ in the transport equation for the Favre mean $\tilde{c}$; it is given [10] by the expression

$$\widetilde{\chi} = \widetilde{\chi}_f = (c_m - \frac{1}{2})\bar{\omega}_c/\bar{\rho} \tag{5}$$

where $c_m = \overline{c\dot{\omega}_c}/\bar{\omega}_c$ and the subscript f signifies combustion in the laminar flamelet burning regime. On the other hand the classical expression [8,13]

$$\widetilde{\chi} = \widetilde{\chi}_t = C_\chi \widetilde{c''^2}\frac{\tilde{\epsilon}}{\tilde{k}} \tag{6}$$

where $\tilde{k}$ and $\tilde{\varepsilon}$ are the turbulent kinetic energy and its dissipation rate, respectively. Eq. (6) provides an adequate description of small scale mixing in nonreactive flows, may also be expected to be applicable to combustion with small heat release and/or at small values of Da. Published models for $\widetilde{\chi}$, whether based on a transport equation [14,15] or an algebraic expression [8,12] do not properly describe the necessary transition between these two limits. If an algebraic model is required, then either the classical nonreactive flow expression of Eq. (6) is assumed to apply or $\widetilde{\chi}$ is assumed [12] to be proportional to $\widetilde{\chi}_f$:

$$\widetilde{\chi} = \widetilde{\chi}_f \frac{\widetilde{c''^2}}{\tilde{c}(1-\tilde{c})} \tag{7}$$

Swaminathan and Bray [16] report progress in this matter, see also [17,18]. They extend the analysis of Mura and Borghi [15] by including effects of dilatation due to heat release and find

$$\widetilde{\chi} = \left(1 + \frac{2}{3}C_{\epsilon c}\frac{s_L^0}{\tilde{k}^{1/2}}\right)\left(C_{Dc}\frac{s_L^0}{\delta_L^0} + C_D\frac{\tilde{\epsilon}}{\tilde{k}}\right)\widetilde{c''^2} \tag{8}$$

at large values of the Damköhler and Reynolds numbers, where s_L^0 and δ_L^0 are laminar burning velocity and flame thermal thickness, respectively, and $C_{\epsilon c}$, C_{Dc} and C_D are model parameters. The ratio of the two factors inside the second brackets in Eq. (8) is proportional to the Damköhler number. If $Da \ll 1$ and $s_L^0/\tilde{k}^{1/2} \ll 1$, Eq. (6) is recovered. On the other hand, when $Da \gg 1$, $\widetilde{\chi}$ is predicted to be proportional to a chemical rate s_L^0/δ_L^0 but the requirement to recover Eq. (5) is not met.

In the present paper it is argued that failure to use an appropriate expression for $\widetilde{\chi}$ can lead to serious errors in both RANS and LES simulations of premixed turbulent combustion. By way of example, consider a presumed pdf analysis [2,3,19], in which the mean rate of reaction is determined by integration over the interior part of the pdf $\widetilde{P}(c;\mathbf{x})$. The classical expression of Eq. (6) predicts too large a value of $\widetilde{\chi}$ in comparison with DNS [16]. Use of this model in the transport equation for the variance $\widetilde{c''^2}$ will underpredict the variance, and thus under-estimate both the interior pdf values and the mean reaction rate. On the other hand, the flamelet expression of Eq. (5) corresponds to a bimodal pdf consisting *only* of two Dirac delta functions situated at $c = 0$ and $c = 1$, respectively. The interior part of the pdf is zero in this limit and a presumed pdf model with finite chemical reaction rates cannot predict a non-zero mean reaction rate. Consequently, at large but finite values of Da, $\widetilde{\chi}$ must be close to $\widetilde{\chi}_f$ but it cannot be equal to $\widetilde{\chi}$.

The aim of the present work is to derive and test an equation to predict the variance factor ϵ_{cc}. In order to do so we must also find an expression for the scalar dissipation $\widetilde{\chi}$ having appropriate limiting behaviour as $Da \to \infty$. It is important to recall here that, in the limit of infinitely thin flamelets, the scalar variance equation degenerates toward the algebraic expression given by Eq. (5). On a numerical point of view such a singular behaviour of the variance equation may preclude its use, for example in CFD codes. Using instead an equation for the more relevant quantity ϵ_{cc}, together with the appropriate form of the scalar dissipation rate, and the appropriate scaling, solves this difficulty. We first derive a general transport equation for ϵ_{cc} and then perform an asymptotic analysis for large values of Damköhler number. The resulting transport equation is applied to the problem of a planar turbulent flame; predictions are compared with data from DNS.

2. Transport equation for ϵ_{cc}

An unclosed transport equation for ϵ_{cc} can be derived from the equations for the variance $\widetilde{c''^2}$ and mean $\tilde{c}$. Derivation of such an equation yields

$$\bar{\rho}\tilde{c}(1-\tilde{c})\left[\frac{\partial \epsilon_{cc}}{\partial t} + \tilde{\mathbf{u}}\cdot\nabla\epsilon_{cc}\right] = \nabla\cdot\mathbf{G} - \epsilon_{cc}(1-2\tilde{c})[\bar{\omega}_c - \nabla\cdot(\bar{\rho}\widetilde{\mathbf{u}''c''})] - (2c_m - 1)\bar{\omega}_c + 2\bar{\rho}\widetilde{\chi} \tag{9}$$

where $\mathbf{G}$ is given by

$$\mathbf{G} = \bar{\rho}[\widetilde{\mathbf{u}''c''^2} - (1-2\tilde{c})\widetilde{\mathbf{u}''c''}] \tag{10}$$

In Eq. (9) the scalar dissipation $\widetilde{\chi}$ can be written in two parts, in terms of the flamelet dissipation $\widetilde{\chi}_f$ and a second contribution $\widetilde{\chi}_t$ which is defined by

$$\bar{\rho}\widetilde{\chi} = (1-\epsilon_{cc})\bar{\rho}\widetilde{\chi}_f + \epsilon_{cc}\bar{\rho}\widetilde{\chi}_t \tag{11}$$

so that $\widetilde{\chi}$ approaches $\widetilde{\chi}_f$ as ϵ_{cc} approaches zero. A more precise expression for $\widetilde{\chi}$ as ϵ_{cc} goes to zero can be obtained by remembering that at the limit $\epsilon_{cc} = 0$ and $\bar{\rho}\widetilde{\chi} = \bar{\rho}\widetilde{\chi}_f = (c_m - 1/2)\bar{\omega}_c$. Then, we write [20]:

$$\bar{\rho}\widetilde{\chi} = (c_m - \frac{1}{2} - \kappa\varepsilon_{cc})\bar{\omega}_c + \epsilon_{cc}\bar{\rho}\widetilde{\chi}_t \quad , \epsilon_{cc} \to 0 \tag{12}$$

where κ is an arbitrary constant of order unity.

For small values of ε_{cc}, i.e. in the bimodal limit corresponding to $Da \gg 1$, Eq. (9) for ϵ_{cc} becomes:

$$\bar{\rho}\tilde{c}(1-\tilde{c})\left[\frac{\partial \epsilon_{cc}}{\partial t} + \tilde{\mathbf{u}}\cdot\nabla\epsilon_{cc}\right] = \nabla\cdot\mathbf{G}(\varepsilon_{cc}\to 0) + \left[(1-2\tilde{c})\nabla\cdot(\bar{\rho}\widetilde{\mathbf{u}''c''}) - 2\left(\frac{1}{2} - \tilde{c} + \kappa\right)\bar{\omega}_c + 2\bar{\rho}\widetilde{\chi}_t\right]\epsilon_{cc} \tag{13}$$

3. Asymptotic analysis for large damköhler numbers

In the limit of large Damköhler numbers we have $\varepsilon_{cc} \to 0$ and $\mathbf{G}(\varepsilon_{cc} = 0) = 0$ as in this bimodal limit we have $\widetilde{\mathbf{u}''c''^2} = (1-2\tilde{c})\widetilde{\mathbf{u}''c''}$. However Eq. (13) requires an expression for the next term in the linear expansion in small ε_{cc}. Such an expression can be derived by considering the pdf $\widetilde{P}(c)$ described as in [4] by

$$\widetilde{P} = \alpha\delta(c) + \beta\delta(1-c) + \gamma\tilde{f}(c) \tag{14}$$

where $\tilde{f}$ is the interior pdf of reactive states. $0 < c < 1$. The three parameters α, β and γ can be expressed as functions of $\tilde{c}$ and $\widetilde{c''^2} = (1-\varepsilon_{cc})\tilde{c}(1-\tilde{c})$. This leads in particular to

$$\gamma = \frac{1}{I_{f1}}\tilde{c}(1-\tilde{c})\varepsilon_{cc} \tag{15}$$

where I_{f1} is a constant integral quantity defined as

$$I_{f1} = \int_{0^+}^{1^-} c(1-c)\tilde{f}dc = I_1 - I_2 \tag{16}$$

where the integral defines the quantities I_1 and I_2.