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Brief Communications

Unclosed Favre-averaged equation for the chemical source and an analytical formulation of the problem of turbulent premixed combustion in the flamelet regime

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1. Introduction

We derive an unclosed Favre-averaged equation that describes the mean chemical source appearing in the combustion equation of the turbulent premixed flame in the flamelet regime. This equation removes the necessity of modelling the surface-averaged variables appearing in the unclosed equation in terms of the flame surface density, Σ, which is used in the literature for estimation of the mean source.

We state an analytical formulation of the turbulent combustion problem including an infinite system of successively derived unclosed equations, which gives a general view of the modelling problem based on the unclosed sub-systems of the infinite system. Although this point seems obvious for the turbulence theory [1], it should be discussed and understood for the analogous situation of turbulent combustion.

We start with the kinematical equation of the instantaneous flame in terms of the progress variable c($c=0$ and $c=1$ in the unburned and burned gases with the densities ρ_u and ρ_b, respectively), which describes an: instantaneous wrinkled laminar flame sheet:

$$\rho\partial c/\partial t+(\rho\vec{u}\cdot\nabla)c=\dot{m}|\nabla c| \tag{1}$$

where $\dot{m}=\rho_u S_L=\rho_b S_L^b=\rho S$ is the flow of mass through a unit area of the thin instantaneous flame per unit time; S_L and S_L^b are the speeds of the flame relative to the unburned and burned gases, and S is the speed relative to an iso-surface $\rho=const$. The specific flux $\dot{m}$ is an invariant characteristic that has the same value for different definitions of the flame speed.

The Favre-averaged combustion equation, which follows from Eq. (1), together with the Favre-averaged mass and momentum hydrodynamics equations, are as follows:

$$\begin{aligned}&\partial\bar{\rho}\tilde{c}/\partial t+\nabla\cdot(\bar{\rho}\vec{\tilde{u}}\tilde{c})+\nabla\cdot\left(\overline{\rho\vec{u}''c''}\right)=\dot{m}\overline{|\nabla c|}\,(=\dot{m}\overline{(\rho(|\nabla c|/\rho)}=\bar{\rho}\tilde{W})\quad(a)\\&\partial\bar{\rho}/\partial t+\nabla\cdot\bar{\rho}\vec{\tilde{u}}=0\quad(b),\\&\partial\bar{\rho}\vec{\tilde{u}}/\partial t+\nabla\cdot(\bar{\rho}\vec{\tilde{u}}\vec{\tilde{u}})+\nabla\cdot(\overline{\rho\vec{u}''\vec{u}''})=-\nabla\bar{p}\quad(c)\end{aligned} \tag{2}$$

The *rhs* term in Eq. (2a) describes the ensemble averaged chemical source, which in brackets is transformed in the Favre-averaged form symbolized as $\bar{\rho}\tilde{W}$, where

$$W=\dot{m}(|\nabla c|/\rho) \tag{3}$$

The unknowns in system (2) are the chemical source $\tilde{W}$ scalar flux $\overline{\rho\vec{u}''c''}$ and stress tensor $\overline{\rho\vec{u}''\vec{u}''}$ ($\bar{\rho}$ is known: $\bar{\rho}=\rho_u/[1+\tilde{c}(\rho_u/\rho_b-1)]$). The unclosed Favre-averaged equation for the flux $\overline{\rho\vec{u}''c''}$ and tensor $\overline{\rho\vec{u}''\vec{u}''}$ are known from the literature and are used for designing advanced models aimed at prediction of the counter-gradient scalar flux and velocity fluctuations in the premixed flame; see for example paper [2]. At the same time, a problem of description of the source with an unclosed equation has no definitive formulation.

The point is that there are two equivalent forms of the mean chemical source:

$$\begin{aligned}&\bar{\rho}\tilde{W}=\dot{m}\overline{|\nabla c|}\quad(a),\\&\bar{\rho}\tilde{W}=\dot{m}\Sigma^*\quad(b)\end{aligned} \tag{4}$$

where $\Sigma^*(c^*)=\overline{|\nabla c|\delta(c-c^*)}$ (the conditional average $|\nabla c|$ for $c=c^*$) [3] is the flame surface density (the mean area of the instantaneous flame area per unit volume). The difference between these two forms is that $\overline{|\nabla c|}(\vec{x},t)$ is defined in the space $(\vec{x},t)$, while $\Sigma^*(\vec{x},t)$ is defined on a particular iso-surface $c=c^*$ (below we omit the index "$*$"). Hence, the unclosed differential equations in terms of $\overline{|\nabla c|}$ and Σ would be ensemble- and surface-averaged equations. The unclosed Σ – equation is known from the literature [3]:

$$\begin{aligned}\partial\Sigma/\partial t+\nabla\cdot(\vec{\tilde{u}}_s\Sigma)=&(\overline{\nabla\cdot\vec{u}}-\overline{\vec{n}\vec{n}:\nabla\vec{u}})_s\Sigma-\nabla\cdot[(\overline{S\vec{n}})_s\Sigma]\\&+(\overline{S\nabla\cdot\vec{n}})_s\Sigma,\end{aligned} \tag{5}$$

where $\vec{n}=-\nabla c(\vec{x},t)/|\nabla c(\vec{x},t)|$ is the unit vector normal to the instantaneous flame pointed towards reactants and $\vec{n}\vec{n}:\nabla\vec{u}=n_in_j\partial u_i/\partial x_j$, and the "$s$" symbol means surface averaging. This equation is defined on a particular iso-surface traveling with the speed S. While Σ is practically the same for all iso-surfaces $\rho_b<\rho<\rho_u$, the surface-averaged velocity $\vec{\tilde{u}}_s$ and speed S change across the instantaneous flame.

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The surface-averaged Eq. (5) is inconsistent with other Favre-averaged equations due to the appearance of surface-averaged speed, $\vec{u}_s$ and other surface-averaged variables, which result in added difficulty regarding their modelling in terms of Favre-averaged variables. We can avoid this problem by directly deducing the Favre-averaged equation in terms of $\tilde{W}$, starting from Eq. (4a). This equation is established in the next section.

2. The Favre-averaged unclosed equation for the mean chemical source

The width of the instantaneous flame is finite; therefore, all instantaneous fields are continuous. At the same time, the width is so small that the values of the mass flux, ρS, through all iso-surfaces inside the instantaneous flame can be assumed to be equal. An equation for the modulus of the progress variable gradient, which follows from Eq. (1) using the equality $\dot{m} = \rho S$ and obvious identities [3]:

$$\begin{aligned} &\partial(|\nabla c(\vec{x},t)|)/\partial t = -\vec{n}\cdot\nabla(\partial c(\vec{x},t)/\partial t) \quad (a)\\ &\partial(|\nabla c(\vec{x},t)|)/\partial x_i = -\vec{n}\cdot\nabla(\partial c(\vec{x},t)/\partial x_i) \quad (b) \end{aligned} \tag{6}$$

is as follows:

$$\partial(|\nabla c|)/\partial t + \vec{u}\cdot\nabla(|\nabla c|) = -|\nabla c|(\vec{n}\vec{n}:\nabla u) - \vec{n}\cdot(\nabla(S|\nabla c|) \tag{7}$$

Introducing the rate of strain acting in the iso-surface tangent plane, $\nabla_t\cdot\vec{u} = \nabla\cdot\vec{u} - \vec{n}\vec{n}:\nabla\vec{u}$, expressing $|\nabla c|$ in terms of W from Eq. (3) and using the equality $\rho S = \dot{m}$, we have the following instantaneous equation in terms of W:

$$\begin{aligned} &\partial(\rho W)/\partial t + \nabla\cdot(\rho\vec{u}W) + \dot{m}\nabla\cdot(\vec{n}W)\\ &\quad = \rho(\nabla_t\cdot\vec{u})W + \dot{m}(\nabla\cdot\vec{n})W \end{aligned} \tag{8}$$

Ensemble averaging of Eq. (8) results in the desired unclosed equation in terms of $\tilde{W}$:

$$\begin{aligned} &\partial(\bar{\rho}\tilde{W})/\partial t + \nabla\cdot(\bar{\rho}\tilde{\vec{u}}\tilde{W}) + \nabla\cdot\overline{\rho\vec{u}''W''} + \dot{m}\nabla\cdot(\overline{\vec{n}W})\\ &= \overline{\rho(\nabla_t\cdot\vec{u})}\tilde{W} + \overline{\rho(\nabla_t\cdot\vec{u})''W''} + 2\dot{m}\overline{KW} \end{aligned} \tag{9}$$

where $K = 0.5\nabla\cdot\vec{n}$ is the curvature of the instantaneous flame and $\dot{m} = \rho_u S_L$.

The lhs of Eq. (9) contains one non-stationary term and three transport terms describing convection by (i) mean velocity transport, (ii) turbulent diffusion-type transport due to correlations of velocity and combustion rate pulsations. and (iii) transport caused by the flamelet movement. Three *rhs* terms describe the effects of different physical mechanisms (sources and sinks) controlling $\tilde{W}$: (i) the flame stretch by the mean velocity field, (ii) the flamelet stretch by the pulsation component of the velocity, and (iii) the effect of the wrinkled flamelet propagation on the sheet area.

The presented direct derivation of the Eqs. (7) and (9) shows that there is no need to invoke the flame surface density concept for chemical source modelling in flamelet premixed combustion. Nevertheless, we note that it is possible to deduce our source equation indirectly (using this concept) with the Σ – equation that is allowed to vary arbitrary through a flamelet region to yield necessary for Favre averaging densities and velocities related to the iso-surfaces $0 \leqslant c^* \leqslant 1$.

3. The analytical formulation of the problem of turbulent premixed combustion

Eqs. (2) and (9) and two Favre-averaged equations for the scalar flux $\overline{\rho\vec{u}''c''}$ and stress tensor $\overline{\rho\vec{u}''\vec{u}''}$ omitted here but found in the literature [2], constitute a set of unclosed self-consistent equations. We could derive the unclosed Favre-averaged equations in terms of all unknowns appearing in the $\overline{\rho\vec{u}''c''}-$ and $\overline{\rho\vec{u}''\vec{u}''}-$ equations, and the $\tilde{W}-$ Eq. (9). Then, in principle, we could derive the unclosed equations in terms of new unknowns appearing in these equations, and so on.

The following total infinite system of equations is closed and it gives an analytical formulation of the problem. This formulation is a generalization of the known analytical formulation in the turbulence theory [1] based on the general method developed by Friedman and Keller for obtaining the differential equations for the moments of arbitrary order [4].

Any finite sub-system of the infinite system is unclosed and needs modelling. The first-order closure models that are normally used in engineering applications are based on the sub-system (2), where the unknown could be modelled assuming, for example, the gradient algebraic expressions for the scalar flux and stress tensor, and algebraic expressions for the chemical source. In the second-order closure models, the scalar flux, stress tensor and chemical source are described by the Favre averaged differential equations, where the appearing unknown terms must be modelled. The Σ – equation cannot be an element of the sub-system as it is defined in the space of the surface averaged functions. Using this equation brings unnecessary difficulties in modelling due to inconsistency between the surface and Favre averaged variables.

An intermediate-order closure model was developed in the cited paper [2], where the scalar flux and stress tensor are described by the differential equations, but at the same time the chemical source is approximated by an algebraic expression. These authors developed recently an approach in terms of the dissipation rate rather than in terms of the flame surface density, where the coefficient in the model expression for the mean chemical source is described by the unclosed differential equation [5].

4. Summary

1. The Favre-averaged unclosed equation is derived in terms of the mean chemical source $\tilde{W}$, this question refers to fundamental issues of the theory of turbulent premixed flame in the flamelet regime. The equation is consistent with others Favre averaged equations for the considered problem, and is an alternative to the surface averaged unclosed Σ – equation that is currently used for modelling the mean chemical source.
2. By analogy to the turbulence theory, we present the analytical formulation of the problem of turbulent premixed combustion, which gives a common vision of the modelling problem, and allows the inconsistency of the surface-averaged equation with other Favre-averaged equations of the problem to be interpreted from a general viewpoint.

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References

[1] A.S. Monin, A.M. Yaglom, Statistical Fluid Mechanics: Mechanics of Turbulence, vol. 1, MIT Press, 1987. p. 9.
[2] K.N.C. Bray, M. Champion, P.A. Libby, Combust. Flame 120 (2000) 1–18.
[3] D. Veynante, L. Vervisch, Progr. Energy Combust. Sci. 28 (2002) 193–266.
[4] L.V. Keller, A.A. Fridman, in: Proc. 1st Intern. Congr. Appl. Mech., Delft, 1924, pp. 395–405.
[5] K.N.C. Bray, M. Champion, P.A. Libby, N. Swaminathan, Scalar dissipation and mean reaction rates in premixed turbulent combustion, Combust. Flame 158 (2011) 2017–2022.