Reaction-Diffusion Equation and G-Equation Approaches Reconciled in Turbulent Premixed Combustion Modelling

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Abstract
Stochastic fluctuations described by an adequate probability density function are imposed to the average flame position in order to give a proper formulation of the flame surface propagation in turbulent premixed combustion. An evolution equation of reaction-difffusion type is derived for an observable that can be understood as the effective burned fraction. When stochastic fluctuations are removed, the G-equation along the motion of the mean flame position is recovered suggesting that approaches based on reaction-diffusion equations and G-equation are indeed complementary and they can be reconciled. Moreover, when a plane front is assumed, the Zimont & Lipatnikov model is recovered. This last result suggests that the proposed equation can be considered as the natural extension of the Zimont & Lipatnikov model to the case with non null mean curvature.

Introduction
Two different approaches are generally adopted in turbulent premixed combustion, namely that one based on a reaction-diffusion equation and that one based on the level-set method. Actually, they are considered alternatives to each other because the solution of the reaction-diffusion equation is generally a continuous smooth function that has an exponential decay, and it is non-zero in an infinite domain, while the level-set method provides a sharp function that is non-zero on a compact domain. However, one of the main results of the present formulation is that these two approaches are indeed complementary and they can be reconciled.

Models based on a reaction-diffusion equation provide the evolution in time and space of the so-called progress variable, which is a scalar field that describes the increasing of the burned fraction. The level-set method is used to describe the evolution of an iso-surface that devides the burned region from the unburned region and it is adopted for the numerical computation of the solution of the so-called G-equation.

Starting from the G-equation that describes the flame surface propagating along the mean flame position, we show that, when stochastic fluctuations are introduced, it is possible to derive a reaction-diffusion equation that describes the effective burned fraction under the assumption that the probability density function (PDF) of the diffusive process underlying the random front motion is known.

Modeling Approach

Let the scalar function $G(\boldsymbol{x},t), \boldsymbol{x}\in\mathbb{R}^n$, be a level surface that represents the front which devides burned and unburned domains and it is denoted by $\Gamma(t), t\geq 0$. Let $\boldsymbol{x_c}$ be a point on the level surface $G=c$ at the instant t_0 , such that the corresponding front is $\Gamma_0=\Gamma(t_0)=\{\boldsymbol{x}=\boldsymbol{x_0}\in S|G(\boldsymbol{x_0},t_0)=c\}$, where $S\subseteq\mathbb{R}^n$. The level surface propagates with a consumption speed given by the laminar burning velocity s_L in the normal direction relative to the mixture element and its evolution is described by the following Hamilton-Jacobi equation where the flow velocity field is $\boldsymbol{u}$

$$\frac{\partial G}{\partial t}+\boldsymbol{u}\cdot\nabla G=s_L\|\nabla G\|. \tag{1}$$

In (1) the propagation in the normal direction is stated by

$$s_L\boldsymbol{n}=-s_L\frac{\nabla G}{\|\nabla G\|}, \tag{2}$$

where $\boldsymbol{n}$ denotes the normal vector.

Let the front motion be described by the random process $\boldsymbol{X_c^\omega}(\hat{\boldsymbol{x}},t)$ where ω labels any independent realization, such that the random contour is

$$\Gamma^\omega(t)=\{\boldsymbol{x}=\boldsymbol{X_c^\omega}(t)\in S|G^\omega(\boldsymbol{X_c^\omega},t)=c\}\ . \tag{3}$$

Let the mean value of $\boldsymbol{X_c^\omega}$ be denoted by $\langle\boldsymbol{X^\omega}(\hat{\boldsymbol{x}},t)\rangle=\hat{\boldsymbol{x}}(t)$, then if $P_c(\boldsymbol{x_c};t|\hat{\boldsymbol{x}})$ is the corresponding PDF, with initial condition $P_c(\boldsymbol{x_c};t_0|\hat{\boldsymbol{x}})=\delta(\boldsymbol{x}-\boldsymbol{x_0})$, the mean flame position is given by the integral

$$\langle \boldsymbol{x_c} \rangle = \int_{\mathbb{R}^n} \boldsymbol{x_c} P_c(\boldsymbol{x_c}; t|\hat{\boldsymbol{x}}) d\boldsymbol{x_c} = \hat{\boldsymbol{x}}(t) \ . \tag{4}$$

Introducing $\check{G}(\hat{\boldsymbol{x}},t)$, with initial condition $\check{G}(\hat{\boldsymbol{x}},t_0)=\check{G}(\boldsymbol{x_0},t_0)=c$, as the implicit formulation of the mean flame position $\hat{\boldsymbol{x}}$, the ensemble averaging of (1) gives

$$\frac{\partial \check{G}}{\partial t} + \hat{\boldsymbol{u}} \cdot \nabla \check{G} = -\widehat{s_L \boldsymbol{n}} \cdot \nabla \check{G} \ . \tag{5}$$

This procedure was previously proposed by Oberlack *et al.* [1].

Since the G-equation can be derived on the basis of considerations about symmetries, there is a unique model for the RHS term of equation (5) providing a relation between the laminar burning velocity s_L and the turbulent burning velocity s_T [1], i.e.

$$\widehat{s_L \boldsymbol{n}} = s_T \check{\boldsymbol{n}}, \qquad \check{\boldsymbol{n}} = -\frac{\nabla \check{G}}{\|\nabla \check{G}\|} \ . \tag{6}$$

Finally, combining equation (5) and model (6), the *G*-equation that describes the surface motion along the mean flame position results to be

$$\frac{\partial \check{G}}{\partial t} + \hat{\boldsymbol{u}} \cdot \nabla \check{G} = s_T \|\nabla \check{G}\| \ . \tag{7}$$

Please, note the difference in (6) between the mean of the normal vectors to the random flame front, i.e. $\hat{\boldsymbol{n}}$, and the normal vector of the mean flame front, i.e. $\check{\boldsymbol{n}}$. In general, we remark here that the mean of the random level surface $\langle G^{\omega} \rangle$ is different from the level surface $\check{G}$ depicted by the mean position of the flame [2].

Applying properties of the Dirac δ-function, we can have an integral formula for the random level surface

$$G^{\omega}(\boldsymbol{X_c^{\omega}}, t) = \int_{\mathbb{R}^n} G(\boldsymbol{x}, t) \delta(\boldsymbol{x} - \boldsymbol{X_c^{\omega}}(\hat{\boldsymbol{x}}, t)) d\boldsymbol{x} \ , \tag{8}$$

and a formula including the stochastic fluctuations around the front depicted by the mean flame position, i.e.

$$\phi^{\omega}(\boldsymbol{x},t)=\int_{\mathbb{R}^n} \check{G}(\hat{\boldsymbol{x}},t)\,\delta(\boldsymbol{x}-\boldsymbol{X}_c^{\omega}(\hat{\boldsymbol{x}},t))\,d\hat{\boldsymbol{x}}\ . \tag{9}$$

We expect that further investigation of the relationships between formula (8) and formula (9) leads to a formula relating $\langle G^{\omega}\rangle$ and $\check{G}$. Presently, we proceed deriving an evolution equation associated to (9).

Given the level surface $\check{G}$, then the inner domain $\check{\Omega}(t)$ enclosed by the front contour $\check{\Gamma}(t)=\{\boldsymbol{x}\in\partial\check{\Omega}(t)\}$ can be understood as the effective volume occupied by the burned fraction. Then the following indicator function is introduced

$$I_{\check{\Omega}}(t)=\begin{cases}1, & \boldsymbol{x}\in\check{\Omega}(t)\\ 0, & \boldsymbol{x}\notin\check{\Omega}(t)\end{cases} \tag{10}$$

In analogy with (9), the random indicator associated to the surfaces which enclose the volume of the burned fraction are given by the following formula

$$\begin{aligned} I_{\check{\Omega}}^{\omega}(\boldsymbol{x},t) &= \int_{\mathbb{R}^n} I_{\check{\Omega}}(\hat{\boldsymbol{x}},t)\,\delta(\boldsymbol{x}-\boldsymbol{X}_c^{\omega}(\hat{\boldsymbol{x}},t))\,d\hat{\boldsymbol{x}} \\ &= \int_{\check{\Omega}} \delta(\boldsymbol{x}-\boldsymbol{X}_c^{\omega}(\hat{\boldsymbol{x}},t))\,d\hat{\boldsymbol{x}}\ . \end{aligned} \tag{11}$$

Finally, ensemble averaging of (11) gives

$$\begin{aligned} \langle I_{\check{\Omega}}^{\omega}(\boldsymbol{x},t)\rangle &= \int_{\check{\Omega}} \langle\delta(\boldsymbol{x}-\boldsymbol{X}_c^{\omega}(\hat{\boldsymbol{x}},t))\rangle\,d\hat{\boldsymbol{x}} \\ &= \int_{\check{\Omega}(t)} P_c(\boldsymbol{x};t|\hat{\boldsymbol{x}})\,d\hat{\boldsymbol{x}}=V_e(\boldsymbol{x},t)\ . \end{aligned} \tag{12}$$

When applying the Reynolds transport theorem to formula (12) we obtain the following evolution equation of reaction-diffusion type

$$\frac{\partial V_e}{\partial t}=\int_{\check{\Omega}(t)} \frac{\partial P_c}{\partial t}\,d\hat{\boldsymbol{x}}+\int_{\check{\Omega}(t)} \nabla_{\hat{\boldsymbol{x}}}\cdot\left[s_T\check{\boldsymbol{n}}\,P_c(\boldsymbol{x};t|\hat{\boldsymbol{x}})\right]d\hat{\boldsymbol{x}}\ . \tag{13}$$

Equation (13) was previously derived with a different argoument in [3].

Considering the general kinetic equation for P_c

$$\frac{\partial P_c}{\partial t} = -\nabla J \ , \tag{14}$$

where J is the flux, equation (13) becomes

$$\frac{\partial V_e}{\partial t} = -\nabla \int_{\check{\Omega}(t)} J(\boldsymbol{x};t|\hat{\boldsymbol{x}})\, d\hat{\boldsymbol{x}} + \int_{\check{\Omega}(t)} \nabla_{\hat{\boldsymbol{x}}} \cdot \left[s_T \check{\boldsymbol{n}} P_c(\boldsymbol{x};t|\hat{\boldsymbol{x}}) \right] d\hat{\boldsymbol{x}} \ . \tag{15}$$

If a flux-gradient relation is assumed, i.e.

$$J(\boldsymbol{x},t) = -D \nabla V_e \ , \tag{16}$$

where D is the diffusion coefficient, equation (15) can be re-written as

$$\frac{\partial V_e}{\partial t} = D \nabla^2 V_e + \int_{\check{\Omega}(t)} \nabla_{\hat{\boldsymbol{x}}} \cdot \left[s_T \check{\boldsymbol{n}} P_c(\boldsymbol{x}-\hat{\boldsymbol{x}};t) \right] d\hat{\boldsymbol{x}} \ , \tag{17}$$

which reduces to a Hamilton-Jacobi equation when no diffusion is assumed [3].

Moreover, when the mean front curvature $\kappa = \nabla \cdot \boldsymbol{n}/2$ is taken into account, and turbulent burning velocity reads $s_T(\boldsymbol{x},t) = s_T(\kappa,t)$, equation (17) becomes

$$\frac{\partial V_e}{\partial t} = D \nabla^2 V_e - \nabla \cdot \int_{\check{\Omega}(t)} s_T \check{\boldsymbol{n}} P_c(\boldsymbol{x}-\hat{\boldsymbol{x}};t)\, d\hat{\boldsymbol{x}}$$

$$+ \int_{\check{\Omega}(t)} P_c \left\{ \frac{\partial s_T}{\partial \kappa} (\nabla_{\hat{\boldsymbol{x}}} \kappa) \cdot \boldsymbol{n} + 2 s_T \kappa \right\} d\hat{\boldsymbol{x}} \ . \tag{18}$$

Hence, if we consider a plane front, such that $\kappa = 0$, we have that $s_T = s_T(t)$ and $\boldsymbol{n} = \boldsymbol{n}(t)$, equation (18) reduces to

$$\frac{\partial V_e}{\partial t} = D \nabla^2 V_e + s_T(t) \left\| \nabla V_e \right\| \ , \tag{19}$$

which is the same equation derived by Zimont & Lipatnikov [4] and studied in [5]. This suggests that equation (18) can be considered as the natural extension of Zimont & Lipatnikov model to the case with non null mean curvature.

Summary and Outlook

In the present extended abstract we have derived an evolution equation of reaction-diffusion type for an observable that can be understood as the effective burned fraction. When stochastic fluctuations are removed, such equation reduces to the G-equation along the motion of the mean flame position, which suggests that approaches based on reaction-diffusion equations and G-equation are indeed complementary and they can be reconciled. Moreover, when a plane front is assumed, the Zimont & Lipatnikov model is recovered. This last result suggests that the proposed equation can be considered as the natural extension of the Zimont & Lipatnikov model to the case with non null mean curvature.

Actually, since the mean contour of the random front is different from the contour depicted by the mean flame position, we expect that further investigation of the proposed observable and the derived equation provide in the future a relationship between these two different descriptions.

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