

A G -Equation Formulation for Large-Eddy Simulation of Premixed Turbulent Combustion

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Introduction

Premixed turbulent combustion in technical devices often occurs in thin flame fronts. The propagation of these fronts, and hence, for instance, the heat release, are governed by the interaction of transport processes and chemistry within the front. In flamelet models this strong coupling is expressed in treating the flame front as a thin interface propagating with a laminar burning velocity s_L . The coupling of transport and chemistry is reflected in the scaling of the laminar burning velocity, which can be expressed as $s_L \sim \sqrt{D/t_c}$, where D is the diffusion coefficient and t_c is the chemical time scale. Flamelet models for premixed turbulent combustion have been extensively used in the past and different models have been formulated for Reynolds averaged and large-eddy simulations (LES).

The G -equation model proposed by Williams [1] is based on the flamelet modeling assumptions and uses a level set method to describe the evolution of the flame front as an interface between the unburned and burned gases. The level set function G is a scalar field defined such that the flame front position is at $G = G_0$, where G_0 is an arbitrary value, and that G is negative in the unburned mixture. The location of G_0 can be defined to be anywhere in the flame, for instance at a given temperature iso-surface. Then, the convection velocity appearing in the G -equation is evaluated at that location, and the laminar burning velocity s_L has to be defined with respect to that location as well. Typically, G_0 is defined to be either immediately ahead of the flame in the unburned, or immediately behind the flame in the burned gases. The burning velocities defined with respect to the unburned and burned are denoted as $s_{L,u}$ and $s_{L,b}$, respectively.

Peters [2–4] has developed an appropriate theory for premixed turbulent combustion describing the corrugated flamelets and the thin reaction zones regimes based on the G -equation formulation. Peters [4] and Oberlack et al. [5] pointed out that, since the G -field has physical meaning only at $G = G_0$, in order to derive the Reynolds averaged G -equation, conventional averaging of the G -field cannot be applied. For LES, this implies that not only is it impossible to obtain a filtered G -field from filtering the instantaneous resolved field, but also that the filter kernels, which are usually being used for filtering the velocity and scalar fields cannot be applied. In the application of the G -equation in LES, these facts have not been considered in the past. Here, we will first develop a new filter kernel that takes information only from the instantaneous resolved flame surface. Thereafter, the equation for the filtered flame front position will be derived. The resulting equation has two unclosed terms, a flame front conditionally averaged flow velocity appearing in the convection term, and the sub-filter burning velocity. To relate the conditional velocity to the unconditionally filtered velocity, which is known from the solution of the momentum equations, a model for this quantity will also be developed. Here, we will develop a G -equation for the filtered flame front position valid in the corrugated flamelets regime. The equation valid in the corrugated flamelets and the thin reaction zones regime, and also a model for the sub-filter burning velocity, will be given in the full paper.

G -Equation for the filtered flame location

Peters [4] and Oberlack et al. [5] have pointed out that for the derivation of a G -equation, describing the ensemble or time averaged flame location, the traditional averaging of the entire G -field cannot be applied.

Because the G -field has physical significance only for $G = G_0$, only the G_0 iso-surface can be of relevance in the averaging procedure. The remaining G -field, which can be defined arbitrarily, must not be used. Instead, Peters [4] has proposed an averaging procedure that only uses the probability density function (pdf) of finding $G = G_0$ at a particular location. This procedure was described only for the one-dimensional case. Oberlack et al. [5] developed a rigorous averaging procedure for the three-dimensional case. Through the consistent application of this averaging procedure, a G -equation for the averaged flame location and an equation for the flame brush thickness have been derived for the corrugated flamelets regime. In this section, we will first develop an appropriate LES filter, and then derive a G -equation for the filtered flame front location in the corrugated flamelets regime by using similar arguments as given by Oberlack et al. [5]. The resulting G -equation will be extended to the thin reaction zones regime in the following section.

A parametric representation of the flame surface \mathcal{F} can be given as

$$\mathbf{x}_f = \mathbf{x}_f(\lambda, \mu, t), \quad (1)$$

where \mathbf{x}_f is the flame front location, and λ and μ are curvilinear coordinates along the flame surface forming an orthogonal coordinate system moving with the flame front. Considering a point P_0 on the flame surface, which is given by the coordinates (λ_0, μ_0) , $\mathbf{x}_f(\lambda_0, \mu_0, t)$ describes the temporal development of the location of the point P_0 in physical space as function of time t . The coordinates λ and μ are hence parameters of the function \mathbf{x}_f and will in the following be written as $\mathbf{\Lambda} = \begin{pmatrix} \lambda \\ \mu \end{pmatrix}$.

For a given set of parameters $\mathbf{\Lambda}$, a spatial filter \mathcal{H} can then be defined as

$$\mathcal{H}(\mathbf{\Lambda} - \mathbf{\Lambda}') = \begin{cases} a(\mathbf{\Lambda}), & \text{if } |\mathbf{x}_f(\mathbf{\Lambda}) - \mathbf{x}_f(\mathbf{\Lambda}')| \leq \frac{\Delta}{2} \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

where Δ is the filter width and $a(\mathbf{\Lambda})$ is a normalization factor that is determined by the normalization condition $\int_{\mathcal{F}} \mathcal{H}(\mathbf{\Lambda} - \mathbf{\Lambda}') d\mathbf{\Lambda}' = 1$. This filter function is substantially different from the conventionally applied filter kernels for scalar quantities. Since the flame is only defined on a surface, the filter also has to move along this surface and cannot be used at an arbitrary point in space. The coordinates used in the filter function are therefore not spatial, but flame surface coordinates. Then, a spatial filtering operation for the flame front location can be defined as

$$\hat{\mathbf{x}}_f(\mathbf{\Lambda}, t) = \int_{\mathcal{F}} \mathbf{x}_f(\mathbf{\Lambda}', t) \mathcal{H}(\mathbf{\Lambda} - \mathbf{\Lambda}') d\mathbf{\Lambda}'. \quad (3)$$

This filtering operation should be described in more detail for clarity. The surface coordinates $\mathbf{\Lambda}$ are defined along the instantaneous flame surface. To obtain the filtered front location, for each point $\mathbf{x}_f(\mathbf{\Lambda})$ on the instantaneous flame surface, the filtering operation Eq. (3) yields a corresponding mean flame front location $\hat{\mathbf{x}}_f(\mathbf{\Lambda})$. These locations define the filtered flame front position. Note, that although $\hat{\mathbf{x}}_f$ is expressed as a function of $\mathbf{\Lambda}$, these parameters are still defined through the unfiltered front.

Applying the filter operation to the equation describing the flame front displacement, which is given by $d\mathbf{x}_f/dt = \mathbf{v} + s_L \mathbf{n}$, leads to

$$\frac{d\hat{\mathbf{x}}_f}{dt} = \hat{\mathbf{v}} + \widehat{s_L \mathbf{n}}, \quad (4)$$

where the conditionally filtered flow velocity $\hat{\mathbf{v}}$ and propagation speed $\widehat{s_L \mathbf{n}}$ are defined in accordance with Eq. (3).

To obtain an equation for the filtered flame front location, the implicit representation of the filtered flame surface, given as

$$\check{G}(\mathbf{x}, t) = G_0, \quad (5)$$

is differentiated and the displacement speed of \check{G} appearing in this equation is associated with the filtered displacement speed of the unfiltered front. This results in

$$\frac{\partial \check{G}}{\partial t} + \frac{d\hat{\mathbf{x}}_f}{dt} \cdot \nabla \check{G} = 0. \quad (6)$$

Note that the $\hat{\cdot}$ -quantities are a direct result of the filtering operation Eq. (3), whereas \check{G} is just the level set representation of the filtered flame front location. Therefore, the filtered flame front is not yet defined by

Eq. (5). Indeed, this equation and its differentiated form could describe any iso-surface. Only by choosing the propagation speed of this surface equal to the filtered propagation speed from Eq. (4), this surface is identified with the filtered flame front location. Introducing Eq. (4) into Eq. (6) yields the G -equation for the mean flame front location as

$$\frac{\partial \check{G}}{\partial t} + \widehat{\mathbf{v}} \cdot \nabla \check{G} = -\widehat{s_L \mathbf{n}} \cdot \nabla \check{G}. \quad (7)$$

As proposed by Oberlack et al. [5], the propagation term $\widehat{s_L \mathbf{n}}$ can be modeled by the turbulent burning velocity, here the sub-grid burning velocity, s_T , and the gradient of the resolved G -field as

$$\widehat{s_L \mathbf{n}} = s_T \check{\mathbf{n}} = -s_T \frac{\nabla \check{G}}{|\nabla \check{G}|}, \quad (8)$$

where $\check{\mathbf{n}}$ is the normal vector of the filtered flame front position

$$\check{\mathbf{n}} = -\frac{\nabla \check{G}}{|\nabla \check{G}|}. \quad (9)$$

Note that according to the definition of G_0 the conditional velocity is either the filtered velocity in the immediate unburned or burned gases, which will be denoted by $\widehat{\mathbf{v}}_u$ and $\widehat{\mathbf{v}}_b$, respectively. Similarly, the turbulent burning velocity has to be defined with respect to the unburned or burned gases, denoted by $s_{T,u}$ and $s_{T,b}$. The following derivations will be made by assuming G_0 to be defined in the immediate unburned. With these notations, Eq. (7) can be written as

$$\frac{\partial \check{G}}{\partial t} + \widehat{\mathbf{v}}_u \cdot \nabla \check{G} = s_{T,u} |\nabla \check{G}|. \quad (10)$$

This equation describes the evolution of the filtered flame front location. To solve Eq. (10), models for the sub-filter burning velocity and the flame front conditioned, filtered velocity have to be provided. The latter quantity has to be modeled in terms of the Favre-filtered velocities, which are known from the solution of the Favre-filtered momentum equations. A model for the conditional velocity will be provided in next section, a model for the sub-filter burning velocity will be given in the full paper.

Model for the conditionally filtered flow velocity

The conditional velocity $\widehat{\mathbf{v}}$ is the velocity at the flame front, weighted with the filter function \mathcal{H} and averaged over the entire flame surface within the filter volume. Physically, this averaged velocity, as it appears in the convection term in Eq. (7), leads to the convection of the entire sub-filter flame surface. Hence, it is important only to capture the large-scale velocity motion in the model for the conditional velocities, and not the small scale velocity fluctuations, which only lead to sub-grid flame wrinkling, but not to convection on the resolved scales. Then, the local unfiltered velocities can be assumed to be constant in the burned and the unburned part of the sub-filter volume. These velocities are then equal to the respective conditional velocities. If G_0 is defined in the unburned, this can be written as

$$\mathbf{v}(G) = \begin{cases} \widehat{\mathbf{v}}_u & \text{if } G \leq G_0 \\ \widehat{\mathbf{v}}_b, & \text{if } G > G_0. \end{cases} \quad (11)$$

The unconditional Favre-filtered velocity can then be expressed by

$$\overline{\rho \mathbf{v}} = \int_{-\infty}^{\infty} \rho \mathbf{v}(G) P(G) dG = \rho_u \widehat{\mathbf{v}}_u \int_{-\infty}^{G_0} P(G) dG + \rho_b \widehat{\mathbf{v}}_b \int_{G_0}^{\infty} P(G) dG, \quad (12)$$

where $P(G)$ is the pdf of finding a particular value of G . Introducing the probability of finding burned mixture as

$$p_b = \int_{G_0}^{\infty} P(G) dG, \quad (13)$$

the unconditional velocity can be written as

$$\bar{\rho}\tilde{\mathbf{v}} = \rho_u\hat{\mathbf{v}}_u(1 - p_b) + \rho_b\hat{\mathbf{v}}_bp_b. \quad (14)$$

Similarly, the unconditionally filtered density can be derived as

$$\bar{\rho} = \rho_u(1 - p_b) + \rho_bp_b. \quad (15)$$

To express $\hat{\mathbf{v}}_b$ by $\hat{\mathbf{v}}_u$, we will use the jump condition for the mass balance across the mean flame interface, given by

$$\rho_u\tilde{\mathbf{n}} \cdot \left(\hat{\mathbf{v}}_u - \frac{\partial \hat{\mathbf{x}}_f}{\partial t} \right) = \rho_b\tilde{\mathbf{n}} \cdot \left(\hat{\mathbf{v}}_b - \frac{\partial \hat{\mathbf{x}}_f}{\partial t} \right). \quad (16)$$

The displacement speed of the mean front can be expressed by Eqs. (4) and (8), where the choice of the conditional velocity and the burning velocity depend on the location of G_0 with respect to the flame. If G_0 is defined to be in the unburned mixture, $\hat{\mathbf{v}}_u$ and $s_{T,u}$ have to be used. For the velocity jump across the flame front this results in

$$\tilde{\mathbf{n}} \cdot (\hat{\mathbf{v}}_u - \hat{\mathbf{v}}_b) = \frac{\rho_u - \rho_b}{\rho_b} s_{T,u}. \quad (17)$$

Introducing Eq. (17) into Eq. (14) results in an expression for the conditional velocity in terms of the unconditional velocity as

$$\tilde{\mathbf{n}} \cdot \hat{\mathbf{v}}_u = \tilde{\mathbf{n}} \cdot \tilde{\mathbf{v}} + \frac{\rho_u - \rho_b}{\bar{\rho}} s_{T,u} p_b. \quad (18)$$

In order to make use of this relation in the G -equation given by Eq. (10), we first split the convection term into a flame normal and a flame tangential part. Since the flame tangential part only leads to a parallel translation of the flame front and has no influence on the flame propagation, it can be neglected. The convection term from Eq. (10) can then be written as

$$\hat{\mathbf{v}}_u \cdot \nabla \check{G} = (\tilde{\mathbf{n}} \cdot \hat{\mathbf{v}}_u) \tilde{\mathbf{n}} \cdot \nabla \check{G}. \quad (19)$$

After introducing Eq. (18) into the normal convection term, only the normal component of the unconditional velocity appears, which can again be complemented by the tangential part without changing the solution. Using Eq. (15), the G -equation for the filtered flame front position can be written as

$$\frac{\partial \check{G}}{\partial t} + \tilde{\mathbf{v}} \cdot \nabla \check{G} = \frac{\rho_u}{\bar{\rho}} s_{T,u} |\nabla \check{G}|. \quad (20)$$

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