

A Joint Probability Density Function (PDF) Model for Turbulent Premixed Combustion

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Abstract

Here, a model for turbulent premixed combustion is presented which is based on a joint probability density function (JPDF) approach. A Lagrangian interpretation of the progress variable from the model by Bray, Moss and Libby (BML) allows to determine the position of the embedded flame front. Furthermore, by introducing a flame residence time τ , the flame structure can be resolved. Numerical simulations show good agreement with experimental data of a turbulent piloted Bunsen flame (Aachen flame F3).

Introduction

In many combustion applications the flow field is highly turbulent, e.g. in gas turbines and internal combustion engines, and reliable models to capture the effects of turbulence, combustion and their interaction are crucial. Various models for non-premixed combustion are based on the mixture fraction, where it is assumed that the inner reactive diffusive flame structure is not disrupted by the turbulence [1, 2, 3]. Such models have proved to be very valuable for the prediction of turbulent diffusion flames [4, 5, 6, 7]. For premixed turbulent combustion, no such general approach exists [8, 9]. In the Eulerian context, a widely used approach for turbulent premixed combustion is the one by Bray, Moss and Libby (BML) [10]. There, a progress variable c is introduced with only two possible states, i.e. 1 for burnt and 0 for unburnt gas. The transport equation for the Favre-averaged progress variable \bar{c} reads

$$\langle \rho \rangle \frac{\partial \bar{c}}{\partial t} + \langle \rho \rangle \bar{U}_i \frac{\partial \bar{c}}{\partial x_i} = - \frac{\partial \langle \rho \rangle \widetilde{u_i'' c''}}{\partial x_i} + \langle \omega_c \rangle \quad , \quad (1)$$

where $\langle \rho \rangle$ is the mean density, \bar{U}_i the Favre-averaged velocity, u_i'' the fluctuating velocity, c'' the fluctuating progress variable and $\langle \omega_c \rangle$ the mean source term of the progress variable. The right hand side of this transport equation, including turbulent convection and mean source term, is unclosed and requires modeling. An alternative modeling approach is the level set method [11, 12] that is based on laminar flamelets, similar as for non-premixed combustion. There, an isosurface of a non-reacting scalar G describes the position of the flame front, for which a transport equation, the so called G-equation, has to be solved. This approach has the advantage that complications due to counter-gradient diffusion are avoided, but it is still not straight forward to achieve closure for turbulent flames.

Here, we present a scale separation model for turbulent premixed combustion [13, 14] that combines the

ideas and advantages of the BML model, the level set approach and of joint probability density function (JPDF) methods [15, 16], where the JPDF is represented by an ensemble of computational particles. The BML model is translated into the Lagrangian JPDF framework, where the progress variable becomes the computational particle property $c^* \in \{0, 1\}$, which acts as a trigger for the arrival of a flame front at the particle location. Note that the asterisk indicates a particle property. Furthermore, to resolve the quasi laminar flame structure, a flame residence time τ^* (the time since the flame arrived at the particle) is introduced for each particle. The remaining challenge is to accurately describe when the flame front reaches the particle, which occurs with the ignition probability P during some time period Δt . Different closure approaches for P are presented and discussed and it is shown that the corresponding transport equation for \bar{c} is consistent with the one by BML. The new framework has the advantage that turbulent convection appears in closed form and it allows a natural description and modeling of turbulent premixed combustion. Numerical simulations of a turbulent premixed piloted Bunsen flame (the Aachen flame F3 [17]) shows good agreement with experimental data.

In the first section, the JPDF method and its numerical implementation is briefly described and in the second section, the combustion model is explained. In the result section, simulation results are presented, validated and discussed; conclusions are given in the last section.

JPDF Method

The mass density function (MDF)

$$\mathcal{G} = \langle \rho \rangle(\mathbf{x}, t) \tilde{g}(\mathbf{v}'', \Psi; \mathbf{x}, t) \quad (2)$$

is the product of the mean density $\langle \rho \rangle$ and the one-point one-time Eulerian mass-weighted JPDF \tilde{g} of the fluctuating velocity $\mathbf{u}'' = (u_1'', u_2'', u_3'')$ and of the composition $\Phi = (\phi_1, \dots, \phi_{N_S+1})$, where \mathbf{v}'' and $\Psi = (\psi_1, \dots, \psi_{N_S+1})$ are the sample space variables of \mathbf{u}'' and Φ , respectively

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(N_s is the number of species). The transport equation of \mathcal{G} can be derived from the Navier Stokes equation and reads

$$\begin{aligned}
\frac{\partial \mathcal{G}}{\partial t} &+ \frac{\partial \mathcal{G} (\widetilde{U}_j - v_j'')}{\partial x_j} - \frac{\partial \widetilde{U}_i}{\partial x_j} \frac{\partial \mathcal{G} v_j''}{\partial v_i''} \\
&+ \frac{1}{\langle \rho \rangle} \frac{\partial \langle \rho \rangle \widetilde{u}_i'' \widetilde{u}_j''}{\partial x_j} \frac{\partial \mathcal{G}}{\partial v_i''} + \frac{\partial \mathcal{G} S_\beta}{\partial \Psi_\beta} \\
&= \frac{\partial}{\partial v_i''} \left(\mathcal{G} \left\langle \frac{1}{\rho} \frac{\partial p}{\partial x_i} - \frac{1}{\langle \rho \rangle} \frac{\partial \langle p \rangle}{\partial x_i} \right. \right. \\
&\quad \left. \left. - \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} + \frac{1}{\langle \rho \rangle} \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} \right|_{\mathbf{v}'', \Psi} \right) \\
&+ \frac{\partial}{\partial \Psi_\beta} \left(\mathcal{G} \left\langle \frac{1}{\rho} \frac{\partial J_i^\beta}{\partial x_i} \right|_{\mathbf{v}'', \Psi} \right) . \quad (3)
\end{aligned}$$

Conditional expectations are denoted as $\langle \cdot | \cdot \rangle$, Reynolds-averaged quantities as $\langle \cdot \rangle$, Favre-averaged quantities as $\bar{\cdot}$ and fluctuations as $''$. Moreover, p is the pressure, ρ the density, τ_{ij} the viscous stress tensor, J_i^β the molecular diffusion flux of species β in the direction of x_i and S_β the source term of species β . The left-hand side of eq. (3) is closed, while the conditional expectations on the right-hand side require modeling. Here, the simplified Langevin model (SLM) is used to close the first term on the right-hand side, whereas for the second right-hand side term a molecular mixing model is required.

Here, the composition vector Φ is expressed as a function of the progress variable c and the residence time τ , and therefore the MDF of fluctuating velocity, turbulence frequency ω , progress variable and residence time, i.e.

$$\mathcal{G} = \langle \rho \rangle (\mathbf{x}, t) \tilde{g}(\mathbf{v}'', \theta, \hat{c}, \hat{\tau}; \mathbf{x}, t) , \quad (4)$$

is considered. Note that θ , \hat{c} and $\hat{\tau}$ are the sample space variables of ω , c and τ , respectively. For the turbulence frequency ω an additional model equation has to be solved [15].

A Lagrangian particle method (PM) is employed to solve the MDF. The particles evolve according to stochastic differential equations and the ensemble density represents \mathcal{G} . Note that \mathcal{G} contains information about the fluctuating, but no information about the mean velocity. Therefore, the Reynolds-averaged Navier-Stokes (RANS) equations are solved simultaneously with a finite volume method (FVM). Thus, we talk about a hybrid particle / finite-volume solution algorithm [18, 19, 20], where the unclosed terms in the RANS equations are closed by extracted moments from the particle ensemble and where the particle method gets the mean velocity from the RANS solution.

PDF-BML Model

The model for turbulent premixed combustion, which is presented here, is based on a scale separation approach

[13, 14]. The idea is based on the model by Bray, Moss and Libby, which is translated into the Lagrangian JPDF context. The progress c^* , which is a computational particle property like the particle position X^* , indicates if the flame front has already reached the particle or not. It has two possible states, i.e. 0 for an unburnt particle and 1 for a burnt one. Note that the mass-weighted PDF \tilde{h} of the progress variable at a given location in space and time can be written as

$$\tilde{h}(c) = (1 - \tilde{c}) \delta(c) + \tilde{c} \delta(1 - c) . \quad (5)$$

Note that the PDF \tilde{h} is fully determined, if the Favre-averaged progress variable is known. An example of such a bimodal PDF is shown in Figure 1.

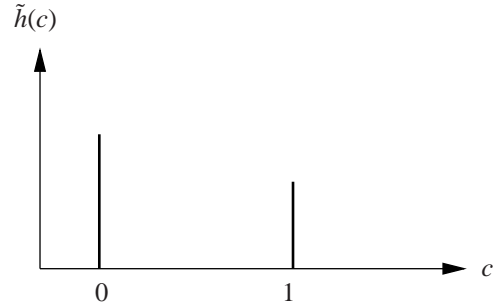


Figure 1: Sketch of a possible bimodal mass weighted PDF \tilde{h} of the progress variable c .

In our scale separation approach, the progress variable is responsible to determine the location of the turbulent flame. Different than in the BML model, however, here a flame residence time τ^* is introduced for each particle. Since it determines the individual time passed since the flame front reached the particle, it allows to resolve the embedded quasi 1D flame profile. Note that this idea is similar to the one used in flamelet modeling of premixed combustion. To decide whether an unignited particle will ignite during a time step, the ignition probability P has to be modeled.

When a particle with $c^* = 0$ at the beginning of the time step ignites (with the probability P), its c^* -value switches to 1. From then on, the residence time τ^* , which was zero so far, gets incremented as the simulation time proceeds. Based on the approximation that the fluid particle evolves along a quasi 1D flame profile, its residence time allows to determine the particle's relative location and thus (from precomputed 1D flames) its composition. Note that these 1D flame profiles depend on the equivalence ratio of the gas mixture.

Figure 2 shows a sketch of the enthalpy profile in a laminar premixed 1D flame. The dashed line indicates the value of c^* , which triggers the beginning of the residence time τ^* and anchors the 1D flame. Since there exists a unique transformation from the τ^* - to the x -space, h^* and other scalars can be retrieved.

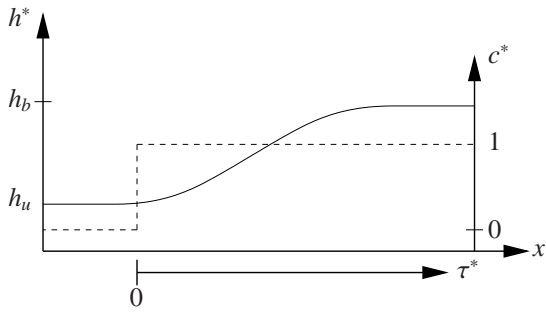


Figure 2: Sketch of the quasi laminar 1D flame profile showing h^* , c^* and τ^* .

The transport equation for the Favre-averaged progress variable derived from the MDF transport equation reads

$$\langle \rho \rangle \frac{\partial \tilde{c}}{\partial t} + \langle \rho \rangle \tilde{U}_i \frac{\partial \tilde{c}}{\partial x_i} = - \frac{\partial \langle \rho \rangle \widetilde{u_i'' c''}}{\partial x_i} + \langle \rho \rangle (1 - \tilde{c}) F \quad , \quad (6)$$

where

$$F = \lim_{\Delta t \rightarrow 0} \frac{P}{\Delta t} \quad . \quad (7)$$

If we set F equal to

$$F = \frac{\langle \omega_c \rangle}{\langle \rho \rangle (1 - \tilde{c})} \quad , \quad (8)$$

we obtain a formulation, which is consistent with the transport equation used in the BML model, i.e. eqs. (1) and (6) become identical. However, other than in the classical BML model, in the PDF context c is not interpreted as a normalized temperature (see explanations above) and the turbulent convection term (first right-hand side term) appears in closed form. The only quantity which requires modeling is F . Here, we employ an ansatz, which was introduced in the BML context, i.e.

$$F = \alpha \langle c \rangle \quad , \quad (9)$$

where α is a variable that may depend on various parameters (note that $P = 1 - e^{-F\Delta t}$, where Δt is the time step size). Therefore, the remaining challenge is to find a general formulation for α . Certainly, it has to capture the influence of the turbulent flow field on the combustion process. In the corrugated flamelet regime, for example, wrinkling of the flame front enhances the turbulent flame speed. As explained above, a possible closure for α can be derived from existing BML models [21, 22, 23]. Alternatively, here the formulation

$$\alpha = C_\alpha(Ka) \omega \quad (10)$$

is employed, where $C_\alpha(Ka)$ is a function of the Karlowitz number Ka . The Karlowitz number $Ka = t_F/t_K$ is defined as the ratio of the chemical time scale t_F and the Kolmogorov time scale t_K and can be determined as

$$Ka = \sqrt{\omega} \sqrt{k} \frac{t_F}{\sqrt{\nu}} \quad . \quad (11)$$

The turbulent kinetic energy $k = \frac{1}{2} \widetilde{u_i'' u_i''}$ is obtained from the particle velocity statistics and the viscosity ν from the composition. Through the dependency of the prefactor on Ka , it is possible to address different turbulent combustion regimes, e.g. for each computational particle one can determine if it belongs to the corrugated, thin reaction zone or broken reaction zone regime. Therefore, the ignition probability can be adjusted correspondingly. A reliable and general formulation of $C_\alpha(Ka)$ will be the topic of future research.

Results

The model for turbulent premixed combustion presented in this paper has been validated for the Aachen flame F3 [17] (a piloted Bunsen flame), which is well documented. A schematic illustration of the axisymmetric flame is shown in Figure 3. There exist three inflow

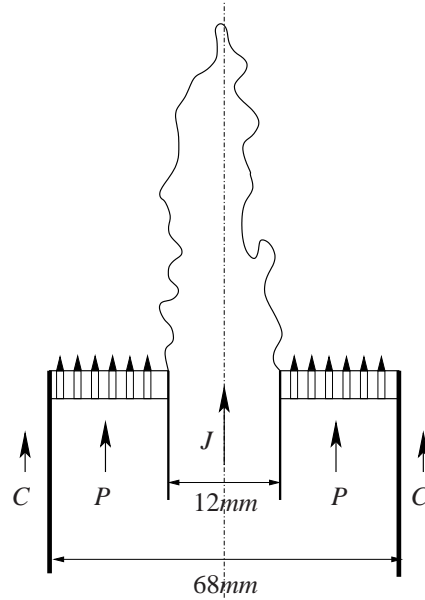


Figure 3: Sketch of the Aachen flame with the unignited jet (J), the hot pilot (P) and the coflow (C).

streams, i.e. in the center the unburnt premixed gas jet, around it the pilot of already burnt premixed gas and outside the surrounding air coflow. The rectangular computational domain is $0.6m$ long in downstream direction (x_1) and $0.1m$ wide in cross-stream direction (x_2). A 50×50 grid is used with 15 particles per cell (in average). At the inflow boundary, \widetilde{U}_1 and the root-mean-square fluctuations $u_{i,rms}$ are directly taken from the measured profiles. The jet bulk velocity is $30m/s$, the mean velocity of the pilot is $1.3m/s$ and the mean coflow velocity is $1.0m/s$. The temperature in the jet and in the coflow is $298K$. In the pilot the temperature is set to $1880K$, since it is water-cooled. In the jet, $\widetilde{u_1'' u_2''}$ is set to be $0.4 u_{1,rms} u_{2,rms}$, and the turbulence frequency ω is determined under the assumption of turbulence in equilibrium.

The ignition probability of a particle is modeled based on a simple formulation for α , which depends only on the

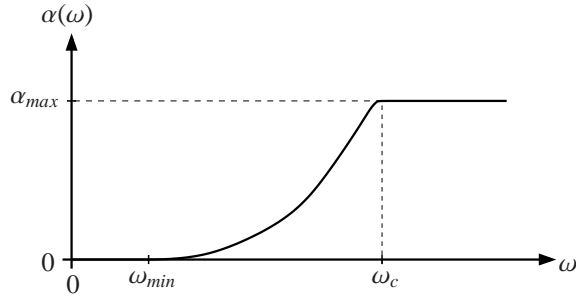


Figure 4: Sketch of $\alpha(\omega)$ used for the simulation studies.

turbulence frequency ω (see Figure 4), i.e.

$$\alpha = H(\omega - \omega_{min}) \min \left\{ \alpha_{max}, \left(\frac{\omega - \omega_{min}}{\omega_c - \omega_{min}} \right)^2 \alpha_{max} \right\}, \quad (12)$$

where $H(\cdot)$ is the Heavyside function. For the present studies, ω_{min} was set to $200s^{-1}$, ω_c to $860s^{-1}$ and α_{max} to $1000s^{-1}$. This dependency of $\alpha(\omega)$ represents the enhancing influence of the turbulence on the turbulent flame propagation in the corrugated flamelet regime, where α is limited by α_{max} .

Normalized mean temperature \hat{T} , normalized mean axial velocity \hat{U} and normalized turbulent kinetic energy \hat{k} are defined as

$$\hat{T} = \frac{\tilde{T} - T_u}{T_b - T_u}, \quad \hat{U} = \frac{\tilde{U}}{U_0}, \quad \hat{k} = \frac{k}{k_0}, \quad (13)$$

where $T_b = 2248K$ is the adiabatic flame temperature, $T_u = 298K$ the temperature of the cold jet, $U_0 = 30 m/s$ the jet bulk velocity and $k_0 = 3.82 m^2/s^2$. Figures 5, 6 and 7 show radial profiles of \hat{U} , \hat{T} and \hat{k} , respectively, at four axial locations, i.e. at $X/D = 2.5, 4.5, 6.5$ and 8.5 ($D = 12 mm$ is the jet diameter). In general, there is very good agreement between the simulation results (solid lines) and the experimental data (dashed lines). At $X/D = 2.5$, the mean temperature is slightly overpredicted (Figure 6), while it is too low at $X/D = 8.5$; like the turbulent kinetic energy.

Conclusions

A new model for turbulent premixed combustion in the PDF modeling context is proposed. The approach is based on a joint PDF method and employs a Lagrangian interpretation of the BML model. Compared to the BML model it has the advantage of closed turbulent convection. Furthermore, the Lagrangian framework allows to introduce a flame residence time, such that the quasi laminar flame structure can be resolved. One possible approach to model the probability P that a computational

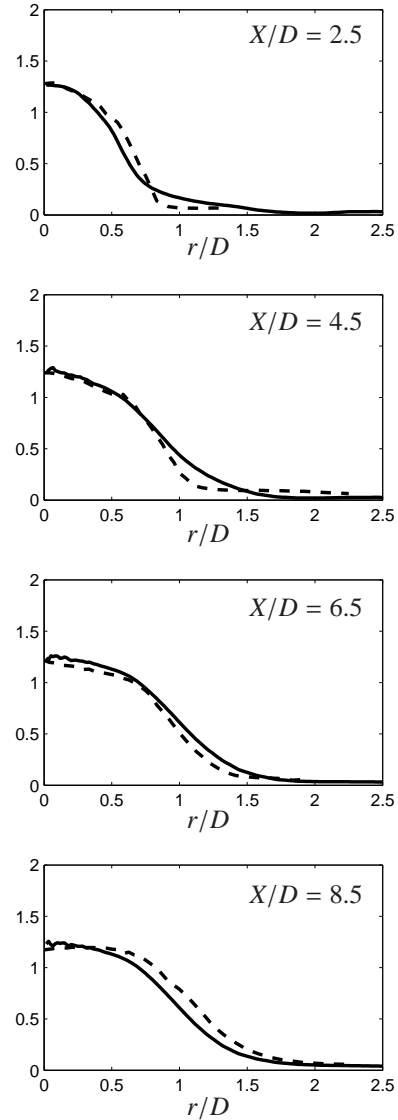


Figure 5: Radial profiles of the normalized mean downstream velocity \hat{U} at several downstream locations (dashed lines: experiments; solid lines: numerical simulation).

particle ignites, is presented; a more general formulation for P is subject of future research. Numerical results of the Aachen flame F3 show very good agreement with the corresponding measurements. Future work will deal with the modeling of more difficult flames, e.g. the Aachen flames F2 and F1, which requires to address the broken reaction zone regime.

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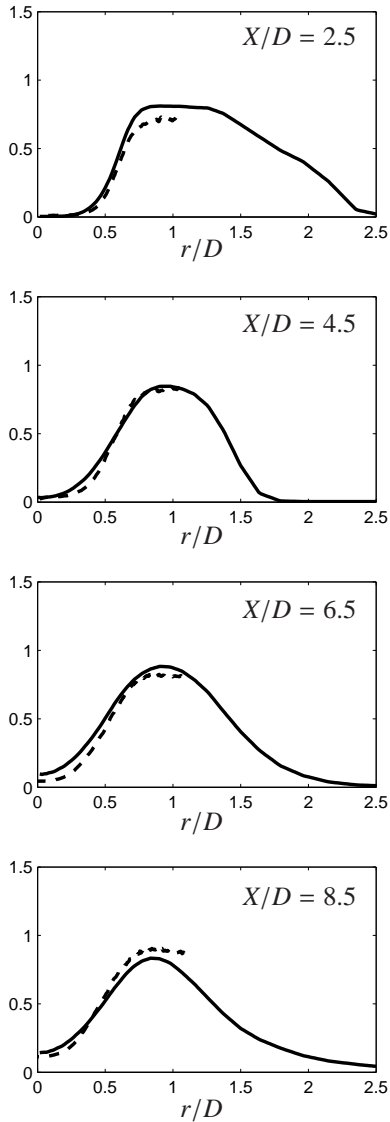


Figure 6: Radial profiles of the normalized temperature \hat{T} at several downstream locations (dashed lines: experiments; solid lines: numerical simulation).

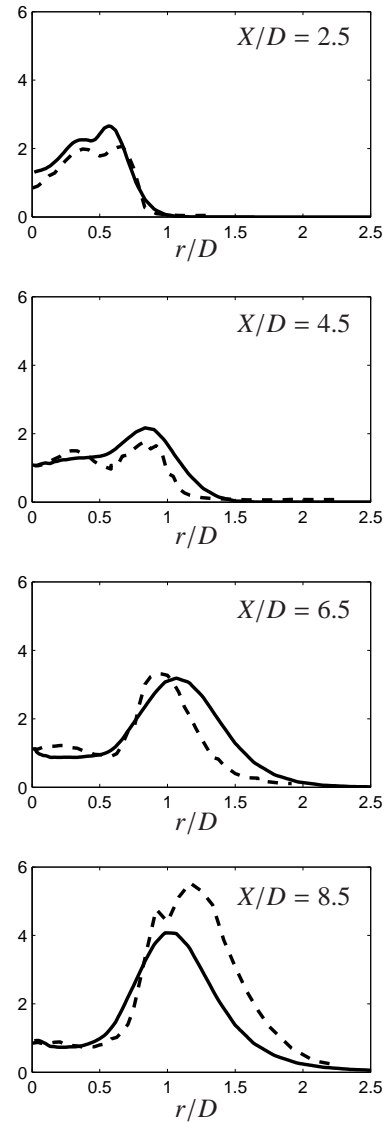


Figure 7: Radial profiles of the normalized turbulent kinetic energy \hat{k} at several downstream locations (dashed lines: experiments; solid lines: numerical simulation).

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