Modeling of Extinction and Re-ignition in Non-premixed Turbulent Combustion

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Unsteady laminar flamelet models are known to have many advantages. However, because of the simplifications made in the derivation of the flamelet equations, the model is not generally valid and fails, for instance, when local extinction and re-ignition events become important.

The influence of the fluctuations of the scalar dissipation rate has recently been investigated by Pitsch and Fedotov [1]. In this work, the flamelet equations are used with the scalar dissipation rate being a random variable. To describe the evolution of the scalar dissipation rate, a stochastic differential equation (SDE) has been formulated. From these two equations a Focker-Plank equation for the joint probability density function of the stoichiometric temperature and the scalar dissipation rate has been derived. It has been shown that the fluctuations of the scalar dissipation rate can have a very strong impact, leading to local extinction, even when the average scalar dissipation rate is below the extinction limit. However, since the study presented in [1] has been based on the flamelet equations, which, as already mentioned, cannot account for re-ignition, the real behavior of the physical system could not be investigated.

In the present work, an extension of the flamelet model is presented, which can account for re-ignition. The resulting modeled equations are solved numerically and the mechanisms of extinction and re-ignition are investigated.

To derive the extended flamelet equations, the equation for the temperature T is considered. The extended flamelet equations for other reactive scalars can be derived similarly. Since the model will subsequently be applied to the results from direct numerical simulations (DNS) we assume constant heat capacity c_p, negligible temporal pressure change and radiative heat loss. The chemistry is described by a one-step reversible reaction with net reaction rate w. A more general formulation accounting for the neglected terms and complex chemistry is a trivial extension of the following derivation. In addition to the temperature equation, we will use the transport equation for the mixture fraction Z below.

We now want to derive a flamelet equation, which accounts for a burning state but also for local extinction and re-ignition processes. In the derivation of the flamelet equations as proposed by Peters [2] starting from the non-dimensional temperature equation, a coordinate transformation of the Crocco-type is performed such that $(t, x_1, x_2, x_3) \longrightarrow (\tau^{\mathrm{o}}, Z, Z_2, Z_3)$, in which the mixture fraction is introduced as a new independent coordinate. This implies that the new coordinate is locally attached to an iso-surface of the mixture fraction, say the stoichiometric mixture fraction Z_{st}, and the new coordinates Z_2, Z_3 lie in this surface. Introducing this transformation into the temperature equation one obtains

$$\rho\frac{\partial T}{\partial \tau^{\mathrm{o}}}-\frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2}-\rho\frac{Q}{c_p}w+\rho\boldsymbol{v}\cdot\nabla_{\perp Z}T-2\nabla Z\cdot\frac{\partial}{\partial Z}\left(\rho D\nabla_{\perp Z}T\right)-\nabla_{\perp Z}\cdot\left(\rho D\nabla_{\perp Z}T\right)-\nabla_{\perp Z}T\cdot\nabla Z\frac{\partial}{\partial Z}\left(\rho D\right)=0\,, \quad (1)$$

where $\nabla_{\perp Z}=(0,\partial/\partial x_2,\partial/\partial x_3)^{\mathrm{T}}$.

In a subsequent asymptotic analysis, Peters shows that changes of the reactive scalars within surfaces of constant mixture fraction are small compared to changes in the direction normal to this surface and can therefore be neglected. This leads to the flamelet equations consisting of the first three terms in Eq. (1)

$$\rho\frac{\partial T}{\partial \tau^{\mathrm{o}}}-\frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2}-\rho\frac{Q}{c_p}w=0\,, \quad (2)$$

where the scalar dissipation rate defined as appears as a new parameter. This equation has been analyzed in DNS of isotropic decaying turbulence with initially non-premixed reactants by Sripakagorn et al. [3]. It has been shown that Eq. (2) describes the extinction process very well, but obviously fails to predict re-ignition. At locations, where local extinction has occurred, the scaling in Eq. (1) changes and the arguments leading to Eq. (2) are no longer true. Terms describing transport within surfaces of constant mixture fraction are then of leading order and therefore have to be considered. After extinction, the maximum flamelet temperature is small and changes in the direction normal to iso-surfaces of the mixture fraction can be neglected. If it is argued that re-ignition occurs by partially premixed flame propagation along iso-surfaces of the mixture fraction, then an asymptotic analysis similar to that of Peters [2] can be performed. Introducing a small parameter as $\varepsilon = l_\mathrm{F}\nabla Z$, where ε represents the ratio of length scales of order unity temperature changes in direction normal to the direction along iso-mixture fraction surfaces, the coordinates Z_2 and Z_3 can be replaced by stretched coordinates such that $\xi_2 = Z_2/\varepsilon$ and $\xi_3 = Z_3/\varepsilon$. Introducing this into Eq. (1) and keeping only leading order terms, the equations describing the re-ignition process are obtained as

$$\rho\frac{\partial T}{\partial \tau^\mathrm{o}} - \nabla_{\perp Z}\cdot(\rho D\nabla_{\perp Z}T) - \rho\frac{Q}{c_p}w = 0\,, \tag{3}$$

where the original coordinates Z_2 and Z_3 have been re-introduced. Since no scaling has been assumed for the time and the reaction term, but it is obvious that these terms are important for re-ignition, these terms have been retained in the equation.

The leading order equation valid to describe both the extinction and the re-ignition process can now be obtained by combining Eqs. (2) and (3) yielding the extended flamelet equation as

$$\rho\frac{\partial T}{\partial \tau^\mathrm{o}} - \frac{\rho\chi}{2}\frac{\partial^2 T}{\partial Z^2} - \nabla_{\perp Z}\cdot(\rho D\nabla_{\perp Z}T) - \rho\frac{Q}{c_p}w = 0\,. \tag{4}$$

In this equation the second term describes the flamelet type diffusive transport, while the third term describes the interaction of different flamelets.

To apply Eq. (4) in a numerical simulation the newly appearing diffusion term has to be modeled. A simple modeling approach is to represent this term by a molecular mixing model frequently used in transported pdf modeling. Using for instance an Interaction by Exchange with the Mean (IEM) model the only remaining modeling problem is the determination of the mixing time T_IEM. This can be done in different ways. A particularly appealing way is to make the assumption that all changes of the temperature along iso-surfaces of the mixture fraction are caused by changes in the scalar dissipation rate. The advantages of this assumption is that it incorporates the fact that extinction is caused by excessive scalar dissipation rate and will also introduce the scalar dissipation rate as a new independent coordinate, which seems reasonable, since the scalar dissipation is the most important parameter in non-premixed combustion.

For the following derivation we first assume that the local instantaneous scalar dissipation rate can be described as a one-parametric function of the mixture fraction $\chi(\boldsymbol{x},t) = \chi_\mathrm{st}(\boldsymbol{x},t)f(Z)$. The exact form of the function $f(Z)$ is not important here.

With this assumption an additional coordinate transformation $\tau^\mathrm{o}, Z, Z_2, Z_3 \longrightarrow \tau^\mathrm{o}, Z, \chi_\mathrm{st}$ can be used to replace the spatial coordinates Z_2 and Z_3 by the scalar dissipation rate and an additional transport term in scalar dissipation rate space is obtained. If this coordinate system is defined such that it moves with a point on the stoichiometric mixture fraction surface the temperature equation can be written as

$$\frac{\partial T}{\partial \tau^\diamond} - \frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2} - \frac{\gamma_\mathrm{st}}{2}\frac{\partial^2 T}{\partial \chi_\mathrm{st}^2} - \frac{Q}{c_p}w = 0\,, \tag{5}$$

where γ_st has been introduced as $\gamma_\mathrm{st} = 2D\left(\nabla\chi_\mathrm{st}\right)^2$. and the scalar dissipation rate has to be introduced as a random parameter.

We now introduce the non-dimensional reaction source term ω and the non-dimensional temperature θ as defined in Ref. [1]. The non-dimensional time and scalar dissipation rate are defined as $\tau = t^*\chi_{\mathrm{st},0}/a$ and $x = \chi/\chi_{\mathrm{st},0}$, where $a = \Delta Z Z_\mathrm{st}\left(1 - Z_\mathrm{st}\right)$ and ΔZ is the reaction zone thickness and $\chi_{\mathrm{st},0}$ is a reference value, here the stoichiometric scalar dissipation rate at extinction.

The temperature equation can then be written as

$$\frac{\partial \theta}{\partial \tau} - \frac{ax}{2}\frac{\partial^2 \theta}{\partial Z^2} - \frac{\Upsilon_\mathrm{st}}{2}\frac{\partial^2 \theta}{\partial x_\mathrm{st}^2} - \omega\left(\theta\right) = 0\,, \tag{6}$$

where $\Upsilon_{\rm st}$ is a dimensionless number representing the ratio of the time scales of the transport in direction of $\chi_{\rm st}$ and the transport in direction of Z and is defined by $\Upsilon_{\rm st} = a\gamma_{\rm st}/\chi^3_{\rm st,0}$. The transport term in direction of Z always causes heat losses away from the reaction zone. In contrast to this, if a locally extinguished spot is considered, the transport term in x-direction leads to a gain of heat from hotter surrounding areas. Hence, $\Upsilon_{\rm st}$ characterizes the ability to re-ignite. Consequently, for $\Upsilon_{\rm st} = 0$ the flamelet equations as given in Ref. [1] are recovered.

Based on the assumption that temperature changes along iso-surfaces of the mixture fraction are only caused by changes in the scalar dissipation rate, we have now derived an equation similar to Eq. (4). However, the present form of the mixing term in $x_{\rm st}$ allows a straightforward physical modeling of the mixing time $T_{\rm IEM}$, if it is expressed by an IEM-model. This leads to

$$\frac{\partial\theta}{\partial\tau} - \frac{ax}{2}\frac{\partial^2\theta}{\partial Z^2} + \frac{\Upsilon_{\rm st}}{2\left\langle x_{\rm st}\right\rangle^2}\frac{\theta - \langle\theta|Z,\Upsilon_{\rm st}\rangle}{C_{\rm IEM}} - \omega\left(\theta\right) = 0\,, \tag{7}$$

where $\langle T|Z,\Upsilon_{\rm st}\rangle$ is the mean temperature conditioned on Z and $\Upsilon_{\rm st}$ of the system at a particular time τ. The mixing time $T_{\rm IEM}$ has been modeled as $T_{\rm IEM} = C_{\rm IEM}\left\langle\chi_{\rm st}\right\rangle^2/\gamma$ and the constant $C_{\rm IEM}$ is set to unity for subsequent numerical simulations.

In Eq. (7), $x_{\rm st}$ and $\Upsilon_{\rm st}$ are fluctuating random quantities. In order to solve Eq. (7) we need to derive SDEs for both. This can be done according to the procedure outlined in Ref. [1]. The resulting equations are

$$dx_{\rm st} = -\frac{x_{\rm st}}{\delta_x}\ln\left(\frac{x_{\rm st}}{\langle x_{\rm st}\rangle}\right)d\tau + \sigma_x\frac{2}{\sqrt{\delta_x}}x_{\rm st}\circ dW_x\left(\tau\right) \tag{8}$$

and

$$d\Upsilon_{\rm st} = -\frac{\Upsilon_{\rm st}}{\delta_\Upsilon}\ln\left(\frac{\Upsilon_{\rm st}}{\langle\Upsilon_{\rm st}\rangle}\right)d\tau + \sigma_\Upsilon\frac{2}{\sqrt{\delta_\Upsilon}}\Upsilon_{\rm st}\circ dW_\Upsilon\left(\tau\right)\,, \tag{9}$$

where dW_x and dW_Υ are independent Wiener processes, δ_x and δ_Υ represent the non-dimensional characteristic time scales of the probability density functions (pdf) of the respective quantity to reach a steady state. σ_x and σ_Υ are the variance parameters of the stationary lognormal pdf.

In order to analyze the influence of the additional term arising in the model, the transport term in Z will be modeled as described in Ref. [1], where also the necessary assumptions are discussed in detail. The equation can then be formulated at $Z_{\rm st}$ leading to

$$\frac{\partial\theta_{\rm st}}{\partial\tau} + x_{\rm st}\theta_{\rm st} + \frac{\Upsilon_{\rm st}}{2\left\langle x_{\rm st}\right\rangle^2}\frac{\theta_{\rm st} - \langle\theta_{\rm st}|\Upsilon_{\rm st}\rangle}{C_{\rm IEM}} - \omega\left(\theta_{\rm st}\right) = 0\,, \tag{10}$$

Assuming that $\Upsilon_{\rm st}$ and $x_{\rm st}$ are constant the steady state solutions of Eq. (10) are easily computed. These solutions are shwon in Fig. 1 for varying $\Upsilon_{\rm st}$. In the case $\Upsilon_{\rm st} = 0$, the well known S-shaped curve is recovered. It is indicated that in the region to the right of the curves, the temporal change of $\Theta_{\rm st}$ is always negative, in the region left of the curves always positive. Hence, if the scalar dissiaption rate is increased beyond the value of the upper turning point, sudden extinction occurs. Re-ignition in this case can only occur, if the scalar dissipation rate decreases to values lower than at the lower turning point, where the temporal temperature change is always positive until the upper steady state is reached. The influence of the diffusion term in χ-space becomes very obvious in the discussion of the steady state solutions for non-zero $\langle\Upsilon_{\rm st}\rangle$. For $\langle\Upsilon_{\rm st}\rangle = 1$ this transport term leads to a heat flux from the hot surroundings to extinguished particles located at the lower steady branch. This additional term hence leads to a shift of the lower turning point to higher scalar dissipation rates. Extinguished particles can therefore re-ignite at much higher values of the scalar dissipation rate. This trend continues for inreasing $\langle\Upsilon_{\rm st}\rangle$. The higher the value of $\langle\Upsilon_{\rm st}\rangle$, the higher the scalar dissipation rate value, which allows for re-ignition. For very large values of $\langle\Upsilon_{\rm st}\rangle$, as shown for $\langle\Upsilon_{\rm st}\rangle = 100$, the turning points of the S-curve and thereby also extinction as well as re-ignition events disappear. Instead, all states on the steady curve are stable.

Monte-Carlo simulations are used to solve the system of equations (10), (8), and (9). For the results presented below, the variance parameters σ and the time scale ratios δ appearing in Eqs. (8) and (9) are all chosen to be unity. For Eq. (8), this choice has been justified in Ref. [1]. All other parameters have been chosen as in Ref. [1]. Three different cases will be shown: $\langle\Upsilon_{\rm st}\rangle$ =1, 10, and 100. In addition, the case

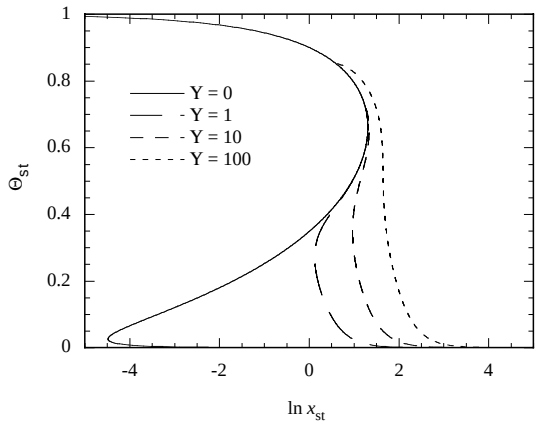

Figure 1: S-curves from steady state solutions of Eq. (10) for different values of $\Upsilon_{st,0}$

$\langle\Upsilon_{st}\rangle = 0$ is shown as reference. This corresponds to the case studied in Ref. [1], where the transport in χ-space does not appear in the flamelet equations.

Numerical results of the system of SDEs are shown in the following figures. In Fig. 2 it is demonstrated that the model presented here is capable of predicting re-ignition. In both figures the paths of some extinguishing notional particals are shown. The left hand side figure is for $\langle\Upsilon_{st}\rangle = 0$, the right hand side figure shows particles with the same x_{st} history, but for $\langle\Upsilon_{st}\rangle = 10$. It has been discussed earlier that for $\langle\Upsilon_{st}\rangle = 0$ re-ignition cannot occur, which can clearly be seen in the left hand side figure. However, in the right hand side it is observed that the extinguishing particles undergo random changes of the scalar dissipation rate. If x_{st} becomes smaller than the respective steady solution, the temporal temperature change becomes positive and the particle can re-ignite.

The pdfs $p(\Theta_{st}, x_{st})$ for $\langle\Upsilon_{st}\rangle = 0$, 1, 10, and 100 are given in Fig. 3. For $\langle\Upsilon_{st}\rangle = 0$ a large amount of particles are extinguished, which can hardly be seen in the figure because of the very narrow distribution at low Θ_{st}. For $\langle\Upsilon_{st}\rangle = 1$ the scalar dissipation rate, where re-ignition can occur is already largely increased. The pdf has similar S-shape as the steady solution curve, but is more pronounced. On the right hand side of the steady state curve, the probability of low temperature is still very high. The reason is that the probability for x_{st} to decrease under the re-ignition value is still very low. At $\langle\Upsilon_{st}\rangle = 10$ the pdf is very similar to the steady state line and the probability of low temperatures strongly decreased. It should be noted that these S-shaped pdfs have also been found in DNS data [3]. At $\langle\Upsilon_{st}\rangle = 100$ extinction can hardly occur and hence there is very low probability to find low temperatures.

Acknowledgements

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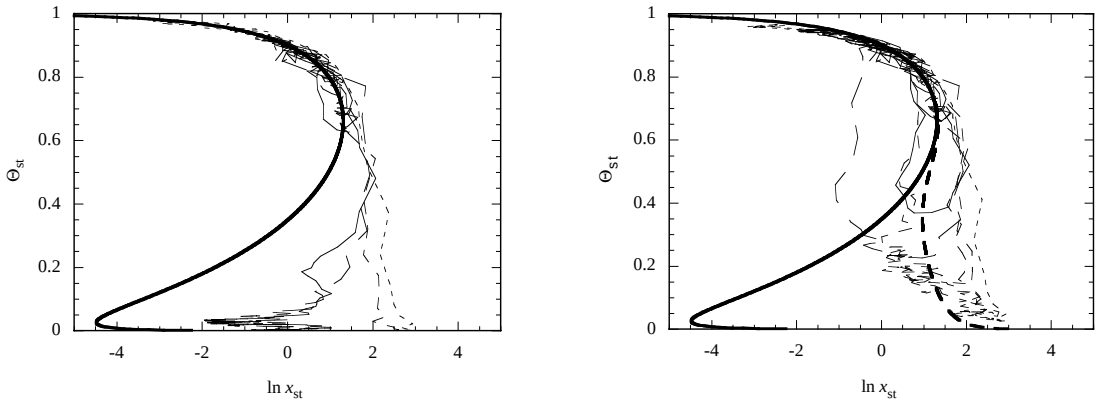

Figure 2: Temporal development of arbitrary extinguishing particles (thin lines). Thick lines are steady state solutions of Eq. (10) for $\langle \Upsilon_{\rm st} \rangle = 0$ (solid line) and $\langle \Upsilon_{\rm st} \rangle = 10$ (dashed line)

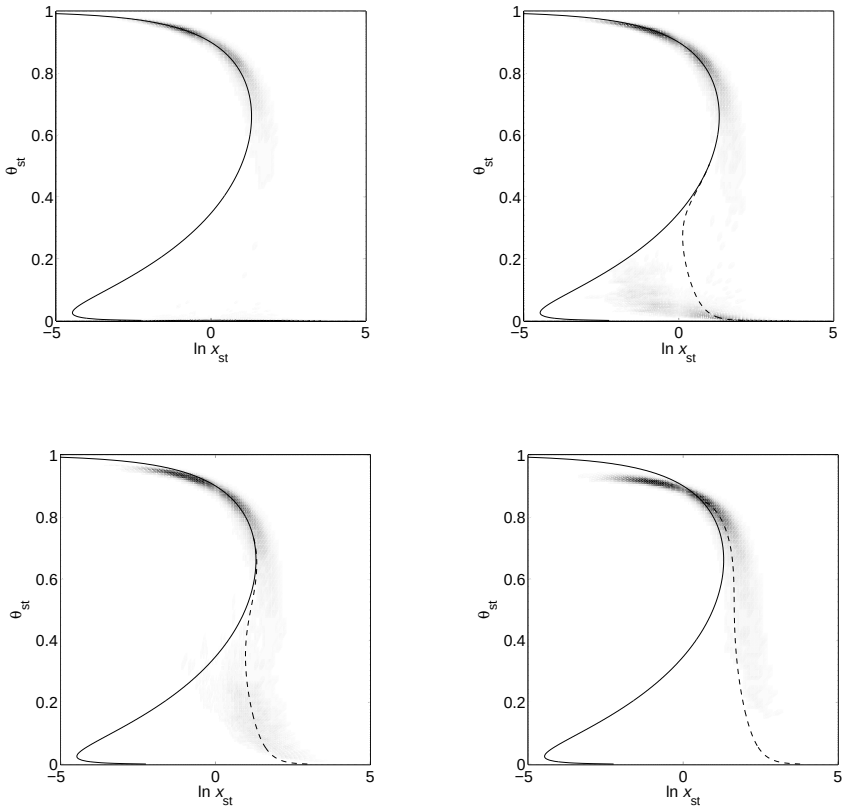

Figure 3: Joint pdfs $p(\Theta_{\rm st}, x_{\rm st})$ for $\langle \Upsilon_{\rm st} \rangle = 0$ (upper left), $\langle \Upsilon_{\rm st} \rangle = 1$ (upper right), $\langle \Upsilon_{\rm st} \rangle = 10$ (lower left), $\langle \Upsilon_{\rm st} \rangle = 100$ (lower right); lines are steady state solutions of Eq. (10) for $\langle \Upsilon_{\rm st} \rangle = 0$ (solid) and $\langle \Upsilon_{\rm st} \rangle = 10$ (dashed)