Numerical Simulation of Turbulent Bunsen Flames with a Level Set Flamelet Model

M. Herrmann

Center for Turbulence Research, Stanford University, CA 94305, USA

Abstract

An extension to the level set flamelet model of Peters [1] for premixed turbulent combustion that takes the effects of cold ambient air entrainment into account is presented. The model is valid in the flamelet regime, where the reaction zone thickness is smaller than the Kolmogorov length scale. The inner structure of the instantaneous flame front is taken into account by a presumed pdf approach of resolved laminar flamelets. To ascertain the performance of the level set flamelet model in an engineering context, the model is coupled to a standard $k$-$\varepsilon$ model describing the turbulent flow field. This RANS level set flamelet model is then applied to the simulation of three turbulent Bunsen flames, F1, F2, and F3, different only in their respective Reynolds numbers. The predicted simulation results are compared to measurements of these flames showing good overall agreement. The results show that all three flames primarily fall within the thin reaction zone regime and that although a significant amount of cold ambient air is entrained close to the turbulent flame front, thereby significantly modifying the composition and the mean temperature of the burned gas flow, the flame front itself burns either in a fully (F3) or almost fully (F1 and F2) stoichiometric premixed environment. Furthermore it is shown that resolving the inner structure of the instantaneous flamelet is a necessity for predicting the mean distribution of certain species, specifically radicals, in the turbulent flame.

Key words: flamelet model, level set, turbulent flames, premixed combustion

1 Introduction

In a wide variety of technical applications turbulent premixed combustion processes occur in the so-called flamelet regime. This regime is characterized by

Email address: Marcus.Herrmann@stanford.edu (M. Herrmann).
reaction zone thicknesses that are smaller than the Kolmogorov length scale. Thus the instantaneous flames essentially burn in a laminar environment and can thus be computationally decoupled from the outside turbulent flow field, precalculated, and then coupled to the turbulent flow field by a presumed pdf approach.

An equation describing the dynamics of a laminar flame front, known as the $G$-equation, has been presented by Williams [2]. It uses the general level set methodology described in Sethian [3] and Osher & Fedkiw [4]. A flamelet model based on the level set formulation for turbulent premixed combustion valid both in the corrugated flamelet regime (the flame thickness is smaller than the Kolmogorov length scale) and the thin reaction zones regime (the reaction zone thickness is smaller than the Kolmogorov length scale) has been derived by Peters [1,5]. This model was applied in conjunction with a RANS turbulence model to a planar turbulent Bunsen flame [1] and to the same three axial-symmetric turbulent Bunsen flames presented here [6]. However, the influence of cold ambient air entrainment was neglected, resulting in significant overpredictions of the temperature and the combustion products in the outer radial regions of the flame.

A variation of the level set flamelet model based on a specific filtering technique that is consistent with the particular symmetries of the level set equation [7], has been proposed by Pitsch [8] within the context of large eddy simulations (LES). They approximate the instantaneous flame front by an infinitely small interface separating unburned from burned gas, thereby neglecting its inner structure. They applied their model to the simulation of two of the three turbulent Bunsen flames presented in this paper, namely F2 and F3, showing good agreement with the experimental data [9] of the flow field and the turbulent kinetic energy profiles, while their temperature profiles are shifted radially inward. However, no flow composition data was presented.

In the RANS context, the flame with the lowest Reynolds number, flame F3, was analyzed by Prasad and Gore [13] using the Bray-Moss model and several different flame surface density models. They compared mean temperature and velocity profiles, finding in general good agreement to the experimental data. However, no mass fraction or turbulent kinetic energy profiles were presented, and neither flame F1 nor F2 were included in the study.

Although LES turbulence models are starting to become the turbulence model of choice in some selected technical applications [10,11], turbulence models based on the Reynolds-averaged Navier-Stokes equations, like the $k\varepsilon$ model, will remain the main turbulence model for industrial technical applications in the near future due to their significantly lower demand on computational resources as compared to LES. Thus, the performance of advanced combustion models, like the level set flamelet model, in conjunction with a relatively simple
turbulence model is still of importance. To this end, we extend the RANS level set flamelet model for premixed turbulent combustion by Peters [1,5] to account for the effect of cold ambient air entrainment into the burned gases and compare its results when solved in conjunction with a standard $k$-$\varepsilon$ model to the experimental data obtained by Chen et al. [9]. This data set contains three different flames denoted F1, F2, and F3 that differ only in their Reynolds number.

Nominally, all three flames, F1, F2, and F3, fall in the regime of thin reaction zones, thus the level set flamelet model is applicable. In the presented model, the inner structure of the instantaneous flame front is taken into account by solving the flamelet equations for premixed combustion. It is shown that for certain species, specifically radicals, resolving the inner structure can have a significant influence on the distribution of their mean mass fractions in the turbulent flame.

In the first part of this paper, the equations of the level set flamelet model for premixed turbulent combustion are reviewed. Then, the numerical methods used in the simulation are briefly summarized. We then present simulation results for first the cold flow case and then the burning case for all three flames F1, F2, and F3. These results are compared to the experimental measurements by Chen et al. [9]. Finally, conclusions are presented.

2 Governing Equations

The turbulent flow field is described by the dimensionless, Favre averaged Navier-Stokes equations in conservative form,

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u}) = 0$$  \hspace{1cm} (1)

$$\frac{\partial \bar{\rho} \bar{u}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{u}) = -\nabla \bar{p} + \nabla \tau - \nabla \cdot \left( \bar{\rho} \bar{u}'' \bar{u}'' \right)$$  \hspace{1cm} (2)

$$\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \nabla \cdot \left[ \left( \bar{\rho} \bar{E} + \bar{p} \right) \bar{u} \right] = \nabla \cdot \left[ \frac{\mu_t}{\text{Pr}_t} \nabla \bar{H} \right] + \tau : \nabla \bar{u},$$  \hspace{1cm} (3)

where $\rho$ is the density, $u$ the flow velocity, $p$ the pressure, $\tau$ the viscous stress tensor, $\rho \bar{u}'' \bar{u}''$ the Reynolds stress tensor,

$$\rho \bar{u}'' \bar{u}'' = \mu_t \left( \nabla \bar{u} + \nabla \bar{u}^T - \frac{2}{3} (\nabla \cdot \bar{u}) \mathbf{I} \right) - \frac{2}{3} \bar{k} \mathbf{I},$$  \hspace{1cm} (4)
\( \mu_t \) the turbulent viscosity,
\[
\mu_t = c_\mu \overline{\rho \frac{k^2}{\varepsilon}}, \quad c_\mu = 0.09, \tag{5}
\]

\( E \) the total energy, \( H \) the enthalpy,
\[
\tilde{H} = \gamma \frac{\bar{p}}{\bar{\rho}} \frac{\tilde{\psi}}{\gamma - 1} + \tilde{\psi}, \tag{6}
\]

\( \text{Pr}_t \) the turbulent Prandtl number, and \( \mathbf{I} \) the identity tensor. The total energy \( \tilde{E} \) is defined as,
\[
\tilde{E} = \frac{\bar{p}}{\bar{\rho}} \frac{\tilde{\psi}}{\gamma - 1} + \frac{1}{2} \tilde{u}^2 + \tilde{k} + \tilde{\psi}, \tag{7}
\]

where \( \gamma = 1.4 \) is the ratio of specific heats and \( \tilde{\psi} \) is the formation enthalpy of the mixture,
\[
\tilde{\psi} = \sum_{i=1}^{N} \tilde{Y}_i h_{i,\text{ref}}. \tag{8}
\]

Here, \( Y_i \) are the mass fractions of the \( N \) species and \( h_{i,\text{ref}} \) are their specific enthalpies. The ideal gas law,
\[
\bar{p} = \bar{\rho} \bar{\Phi} \tilde{T}, \tag{9}
\]

with \( \tilde{T} \) the temperature, \( \bar{\Phi} \) the gas constant of the mixture,
\[
\bar{\Phi} = \mathcal{R} \sum_{i=1}^{N} \frac{\tilde{Y}_i}{W_i}, \tag{10}
\]

\( \mathcal{R} \) the universal gas constant, and \( W_i \) the molecular weight of species \( i \), closes the system of equations.

In order to take partial premixing and dilution effects into account, the mixture fraction \( Z \) is introduced, ranging from 0 in pure air to 1 in the fuel stream. Note that in the flames analyzed in this paper, the fuel stream is stoichiometric, thus \( Z = 1 \) represents a stoichiometric mixture. The equation for the mean of \( Z \),
\[
\frac{\partial \bar{\rho} \bar{Z}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{Z}) = \nabla \cdot \left[ \frac{\mu}{S_{clZ}} \nabla \bar{Z} \right]\]
is solved together with the equation for its variance,
\[
\frac{\partial \tilde{\rho} \tilde{Z}''}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{Z}''^2) = \nabla \cdot \left[ \frac{\mu_t}{Sc} \nabla \tilde{Z}' \right] + \frac{2\mu_t}{Sc \tilde{Z}''} (\nabla \tilde{Z})^2 - \tilde{\rho} \tilde{\chi},
\tag{12}
\]
where all Schmidt numbers are chosen as 0.7 and the scalar dissipation rate \(\tilde{\chi}\) is modeled as
\[
\tilde{\chi} = c_{\chi} \frac{\tilde{\varepsilon} \tilde{Z}''^2}{k}, \quad c_{\chi} = 2.0.
\tag{13}
\]
A standard \(k-\varepsilon\) turbulence model employing a correction term by Pope for swirl free axial symmetric flows is used [14],
\[
\frac{\partial \tilde{\rho} \tilde{k}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{k}) = \nabla \cdot \left( \frac{\mu_t}{Pr_k} \nabla \tilde{k} \right) - \tilde{\rho} \tilde{u}'' \tilde{u}' : \nabla \tilde{u} - \tilde{\rho} \tilde{\varepsilon}
\tag{14}
\]
\[
\frac{\partial \tilde{\rho} \tilde{\varepsilon}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{\varepsilon}) = \nabla \cdot \left( \frac{\mu_t}{Pr_\varepsilon} \nabla \tilde{\varepsilon} \right) - c_{\varepsilon_1} \frac{\tilde{\varepsilon}}{k} \tilde{\rho} \tilde{u}'' \tilde{u}' : \nabla \tilde{u} + (c_{\varepsilon_3} \tilde{\chi}_v - c_{\varepsilon_2}) \frac{\tilde{\rho} \tilde{\varepsilon}^2}{k},
\tag{15}
\]
with the vortex stretching invariant \(\tilde{\chi}_v\),
\[
\tilde{\chi}_v = \frac{1}{4} \left( \frac{k}{\varepsilon} \right)^3 \left( \frac{\partial \tilde{u}_1}{\partial r} - \frac{\partial \tilde{u}_2}{\partial x} \right)^2 \frac{\tilde{u}_2}{r}.
\tag{16}
\]
The model constants are \(Pr_k = 1.0, Pr_\varepsilon = 1.3, c_{\varepsilon_1} = 1.44, c_{\varepsilon_2} = 1.92,\) and \(c_{\varepsilon_3} = 0.79.\)

In the level set framework, the location of the instantaneous flame front is given by the iso surface \(G = G_0\) of the level set scalar \(G\). The evolution equation for this iso surface, the so called \(G\)-equation [15], can be derived from simple kinematic considerations,
\[
\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = s_L |\nabla G|,
\tag{17}
\]
where \(s_L\) is the laminar burning velocity.

A \(G\)-equation describing the location of the averaged flame front \(\tilde{G} = G_0\) both for the corrugated and the thin reaction zones regime was derived by Peters [1,5]. It should be pointed out, that since Eq. (17) has physical significance only at \(G = G_0\), traditional averaging procedures cannot be applied to derive
an evolution equation for the mean flame position. Instead, either averaging procedures limited only to the flame surface \( G = G_0 \) developed for example by Oberlack et al. [7] and Pitsch [8], or averaging procedures that use only the probability density function (pdf) of finding \( G = G_0 \) as used by Peters [1] have to be employed. The latter approach is used here, yielding a transport equation for both \( \tilde{G} \) and its variance \( \tilde{G}^{\prime\prime2} \),

\[
\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \bar{\rho} \bar{u} \cdot \nabla (\tilde{G}) = (\bar{\rho} s_T) |\nabla \tilde{G}| - \bar{\rho} D_t \tilde{\kappa} |\nabla \tilde{G}| ,
\]

(18)

\[
\bar{\rho} \frac{\partial \tilde{G}^{\prime\prime2}}{\partial t} + \bar{\rho} \bar{u} \cdot \nabla (\tilde{G}^{\prime\prime2}) = \nabla_{||} \cdot ((\bar{\rho} D_t \nabla_{||} \tilde{G}^{\prime\prime2}) + 2 \bar{\rho} D_t (\nabla \tilde{G})^2 - c_s \bar{\rho} \tilde{G}^{\prime\prime2} ,
\]

(19)

where \( s_T \) is the turbulent burning velocity, \( D_t \) the turbulent diffusivity, \( \tilde{\kappa} \) the curvature of the mean flame front,

\[
\tilde{\kappa} = - \left[ \nabla \cdot \left( \frac{\nabla \tilde{G}}{|\nabla \tilde{G}|} \right) \right]_{\tilde{G} = G_0} ,
\]

(20)

\( c_s \) a modeling constant \( c_s = 2.0 \) [5], and \( \nabla_{||} \) denotes differentiation in the mean flame front tangential direction.

Note, that Eqs. (18) and (19) are valid only at \( \tilde{G} = G_0 \). Hence, to make \( \tilde{G} \) and \( \tilde{G}^{\prime\prime2} \) quantities defined in the whole field, suitable extensions to \( \tilde{G} \neq G_0 \) have to be employed. To this end, \( \tilde{G} \) is defined as a distance function, ie.

\[
|\nabla \tilde{G}| = 1
\]

(21)

and \( \tilde{G}^{\prime\prime2} \) is kept constant in the flame normal direction,

\[
\nabla \tilde{G}^{\prime\prime2} \cdot \nabla \tilde{G} = 0 .
\]

(22)

By enforcing Eq. (22), the additional normal transport term in the \( \tilde{G}^{\prime\prime2} \)-equation found by Oberlack et al. [7] is not necessary, since due to Eq. (22) all normal transport terms in Eq. (19) are by definition zero.

The turbulent burning velocity in partially premixed environments \( s_T \) can be expressed in terms of the laminar burning velocity \( s_L \) by [1,12]

\[
\bar{\rho} s_T = \int_{0}^{\infty} \int_{0}^{1} \rho(Z)s_L(Z, K) (1 + \tilde{\sigma}_t(Z)) P(Z) P(K) dZdK \bigg|_{\tilde{G} = G_0} ,
\]

(23)
conditioned on $\tilde{G} = G_0$, where $\tilde{\sigma}_t$ is the ratio of flame surface area increase due to turbulence and $P(\tilde{Z})$ and $P(K)$ are the probability density functions for the mixture fraction $Z$ and the stretch rate $K$ respectively. Here, for simplicity, we will assume that both $P(\tilde{Z})|\tilde{G}=G_0$ and $P(K)|\tilde{G}=G_0$ are delta functions. Strictly speaking, $P(\tilde{Z})$ ought to be a beta function pdf, however, in the calculations presented in this paper, $\tilde{Z}|\tilde{G}=G_0 \approx 1$ and $\tilde{Z}'^2|\tilde{G}=G_0 \approx 0$, compare Fig. 9, justifying the choice of a delta function pdf for $P(\tilde{Z})|\tilde{G}=G_0$ to calculate the turbulent burning velocity. Equation (23) then reduces to

$$s_T(\tilde{Z}, \tilde{K}) = s_L(\tilde{Z}, \tilde{K}) \cdot (1 + \tilde{\sigma}_t),$$

with the mean stretch rate calculated from

$$\tilde{K} = \tilde{\varepsilon}/\kappa.$$

The transport equation for $\tilde{\sigma}_t$ valid in both the corrugated flamelet and the thin reaction zone regime was derived by Peters [5], yielding

$$\tilde{\rho} \frac{\partial \tilde{\sigma}_t}{\partial t} + \tilde{\rho} \tilde{u} \cdot \nabla \tilde{\sigma}_t = \nabla || \cdot (\tilde{\rho} D_t \nabla || \tilde{\sigma}_t) + c_0 \tilde{\rho} \frac{u'' u''}{k} \tilde{\sigma}_t + c_1 \tilde{\rho} D_t \frac{(\nabla \tilde{G})^2}{G''^2} \tilde{\sigma}_t - c_2 \frac{\tilde{\rho} s_L}{G''^2} \tilde{\sigma}_t^2 - c_3 \frac{\tilde{\rho} D}{G''^2} \tilde{\sigma}_t^3.$$

(26)

Here, the terms on the left-hand side describe unsteady change and convective transport, whereas the terms on the right-hand side denote turbulent transport, production of flame surface area by mean velocity gradients, turbulent production, kinematic restoration, and scalar dissipation of flame surface area. The modeling constants in Eq. (26) are $c_0 = 1 - c_1 = 0.44$, $c_1 = 4.63$, $c_2 = 1.01$, and $c_3 = c_1 = 4.63$ [1,5]. All modeling constants follow from the derivation of the model and the limit of turbulent production equals kinematic restoration and scalar dissipation for steady planar flames [1,5]. The exception is $c_1$, which was determined from DNS of the constant density $G$-equation in homogenous isotropic turbulence [16]. The diffusivity $D$ is calculated from a reference laminar burning velocity $s_{L,\text{ref}}$ and a reference flame thickness $l_{F,\text{ref}}$,

$$D = s_{L,\text{ref}} l_{F,\text{ref}} = 1 \cdot 10^{-4} \text{ m}^2/\text{s}.$$

(27)

Again, since $\tilde{\sigma}_t$ has physical meaning only at $\tilde{G} = G_0$, $\tilde{\sigma}_t$ has to be extended to $\tilde{G} \neq G_0$ by keeping it constant in the flame normal direction,

$$\nabla \tilde{\sigma}_t \cdot \nabla \tilde{G} = 0.$$

(28)
Finally, a flamelet approach is used to calculate both the chemical composition of the mixture and hence its formation enthalpy and gas constant, as well as the laminar burning velocity. Within the flamelet approach, the averaged turbulent flame front is viewed as an ensemble average of laminar flame structures, the so-called flamelets. Both in the corrugated flamelet and the thin reaction zones regime, chemistry occurs at length scales smaller than the smallest turbulent length scales. Thus, the calculation of the flame’s instantaneous chemical structure can be decoupled from the outside turbulent flow calculation.

Performing a two scale asymptotic analysis of the reacting Navier-Stokes equations, the flamelet equations describing the laminar flame structure can be derived [1,17],

\[
\frac{\partial \rho Y_i}{\partial t} + \frac{\partial (\rho s_L Y_i)}{\partial x_n} = \frac{\partial}{\partial x_n} \left( \rho D_i \frac{\partial Y_i}{\partial x_n} \right) + \omega_i - \rho K Y_i .
\]  

(29)

Here, \( \omega \) is the chemical source term and \( K \) is the stretch rate [18].

Solving the flamelet equations for a given \( K \) and \( Z \) gives the laminar burning velocity \( s_L \) and the mass fractions \( Y_i \) as a function of the coordinate \( x_n \) through the flamelet, with \( x_n = 0 \) defined to be the position of the inner layer temperature. Fixing also the iso surface of the instantaneous flame front \( G = G_0 \) to the position of the inner layer then yields

\[
x_n = \frac{G - G_0}{\sigma} ,
\]  

(30)

with \( \sigma = |\nabla G| \).

Employing the presumed shape pdf approach, the mean mass fraction \( \bar{Y}_i \) can then be calculated from

\[
\bar{Y}_i(x, t) = \int_0^1 \int_{-\infty}^{\infty} \int_{0}^{\infty} Y_i \left( \frac{G - G_0}{\sigma}, Z, K, t \right) P(Z, G, \sigma, K; x, t) dK d\sigma dG dZ .
\]  

(31)

Assuming delta function pdfs for both \( \sigma \) and \( K \), independence of \( Z \) and \( G \) in \( P(Z, G) \), and using Eq. (30), Eq. (31) reduces to

\[
\bar{Y}_i(x, t) = \int_0^1 \int_{-\infty}^{\infty} Y_i(x_n, Z, \bar{K}, t) P(Z; x, t) P(x_n; x, t) dx_n dZ .
\]  

(32)

Here, a standard beta-function pdf is employed to approximate \( P(Z) \), and, according to experimental data [19], the probability density of finding an in-
stantaneous flame front at a given point in space $x$ and time $t$ can be described by a Gaussian distribution. Thus,

$$
P(x_n; x, t) = \frac{1}{(2\pi x_n^{n2})^{1/2}} \exp\left(-\frac{(x_n - \bar{x}_n)^2}{2x_n^{n2}}\right) \quad (33)
$$

with

$$
\bar{x}_n = \bar{G}/\bar{\sigma}, \quad \bar{x}_n^{n2} = \bar{G}'^2/\bar{\sigma}^2. \quad (34)
$$

In conclusion, the following set of ten differential equations, consisting of Eqs. (1)-(3), (11), (12), (14), (15), (18), (19), and (26) are solved to calculate the turbulent Bunsen flames presented in this paper. This flamelet model represents an extension of the premixed flamelet model by Peters [1,5] taking the effect of entrainment of cold ambient air into the burned gases into account.

3 Numerical Methods

All transport equations, ie. Eqs. (1)-(3), (11), (12), (14), (15), (18), (19), and (26) are solved using an operator splitting technique by Strang [20]. The convection operator is solved using a Godunov type method with an approximate Riemann solver by Roe [21] achieving second-order accuracy with a method by Yee et al. [22]. The diffusion operator uses central differencing and a two step Runge-Kutta algorithm. All source terms are integrated in time by evaluating their analytically derived solution [6].

All variables are defined at cell-centers. Thus, any centerline singularity is avoided. Since the calculated mean flame front geometries are smooth and do not exhibit any significant corrugations, a standard 9 point stencil is employed to evaluate the curvature term appearing in Eq. (18).

The reinitialization condition (21) is solved by first reconstructing the $\bar{G} = G_0$ interface shape by line segments in each computational cell, where the cell face cut points are determined by third-order polynomials. Then, the minimum of the distance from a given node to each of these line segments is the solution to Eq. (21). Although this approach is computationally expensive, it exhibits less undesired movement of the $\bar{G} = G_0$ front when solving Eq. (21) by an iterative procedure, for example the one proposed by Sussman et al. [23].

The redistribution conditions (22) and (28) are also solved by a geometric approach [6]. Here, for every grid node close to $\bar{G} = G_0$, the local normal
vector $\tilde{n}$,

$$\tilde{n} = \frac{\nabla \tilde{G}}{|\nabla G|},$$  \hspace{1cm} (35)

is followed to find the corresponding base point on $\tilde{G} = G_0$. That value of $\tilde{G}^{\tilde{n}}$ respectively $\tilde{\sigma}_t$ is then assigned to the node. Again, this approach is computationally expensive, but it avoids any possible errors introduced by an iterative scheme, for example the one proposed by Peng et al. [24].

The stoichiometric laminar flamelet libraries ($Z = 1$) are precalculated by the flamelet solver chem1d [25] solving Eq. (29) using the GRI-MECH 3.0 mechanism [26]. Neumann boundary conditions are used at the burned side boundary and stoichiometric mixture at $T = 300$ K is introduced at the unburned boundary. The stretch rate is successively increased from the non-stretched case $K = 0$, up to $K = K_q = 2806 \text{s}^{-1}$, where quenching of the stoichiometric premixed flamelet occurs.

In the three flames analyzed in this paper, mixing with the cold ambient air ($Z = 0$) occurs predominantly with the fully burned gases. Thus the instantaneous composition is determined by

$$Y_i(Z, K, x_n) = Y_{i,\text{air}} + Z \cdot (Y_i(Z_{st}, K, x_n) - Y_{i,\text{air}}),$$ \hspace{1cm} (36)

where $Y_{i,\text{air}}$ are the mass fractions of species $i$ for pure air. However, the potential influence of the ambient air on the laminar burning velocity $s_L(Z, K)$ is captured, by determining $s_L$ from diluted, stretched, premixed flamelets, see Fig. 1. For $K > K_q$ the laminar burning velocity is set to $s_L = 0$, while the

Fig. 1. Flamelet library laminar burning velocity $s_L(Z, K)$ for $K = 0 \text{s}^{-1}$ (––), $K = 702 \text{s}^{-1}$ (–○–), $K = 1403 \text{s}^{-1}$ (–▲–), $K = 2104 \text{s}^{-1}$ (–▲–), $K = 2806 \text{s}^{-1}$ (–■–)

mass fraction distributions are taken from the last burning flamelet, $K < K_q$. This approach models extinction and re-ignition only very crudely. If $K > K_q$ the flame simply does not propagate normal to itself anymore but retains
its chemical structure. If $K$ drops again below $K_q$, burning is again initiated directly by now taking a non-zero value of the burning velocity.

The pdf integration (32) is precalculated and stored together with $\tilde{\psi}$, Eq. (8), $\Phi$, Eq. (10), and $s_L(\tilde{Z}, \tilde{K})$ in look-up tables that are accessed by the flow solver. In order to speed up this access, the distribution of library node coordinates are determined by either linear distribution, as is the case for the $\tilde{K}$, $\tilde{Z}$, and $\tilde{Z}^{n2}$ coordinates, or two quadratic distributions, as is the case for the $\tilde{x}_n$ and the $\tilde{x}_n^{m2}$ coordinates. This allows for a direct access into the library, with the final library value being calculated by linear interpolation between bracketing library nodes. The employed library resolution is 5 nodes in the $\tilde{K}$-direction, 10 nodes in the $\tilde{Z}$-direction, 5 nodes in the $\tilde{Z}^{n2}$-direction, 175 nodes in the $\tilde{x}_n$-direction, and 40 nodes in the $\tilde{x}_n^{m2}$-direction.

The effect of using finite rate chemistry by resolving the flamelet structure by Eq. (29) as compared to infinitely fast chemistry for the premixed flame is summarized in Fig. 2 showing the mean mass fraction of OH as a function of $\tilde{G}$ for a planar turbulent flame with varying turbulent intensities $u'/s_L$ and $\ell/l_{F,ref} = 10$, where $\ell$ is the integral length scale. As can be clearly seen, the influence can be quite significant near the location of the mean flame front, while both methods converge to the same solution further away in the burned region.

4 Results

We present results obtained with the RANS level set flamelet model for the three axial symmetric turbulent stoichiometric methane-air Bunsen flames studied by Chen et al. [9]. These flames differ only in their Reynolds number, with $Re = 52000$ for flame F1, $Re = 40000$ for flame F2, and $Re = 24000$.
Global operating characteristics of the investigated turbulent Bunsen flames

Table 1

<table>
<thead>
<tr>
<th>Flame</th>
<th>F1</th>
<th>F2</th>
<th>F3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>52000</td>
<td>40000</td>
<td>24000</td>
</tr>
<tr>
<td>$u_0$ [m/s]</td>
<td>65</td>
<td>50</td>
<td>30</td>
</tr>
<tr>
<td>$k_0$ [m$^2$/s$^2$]</td>
<td>12.70</td>
<td>10.80</td>
<td>3.82</td>
</tr>
<tr>
<td>$\varepsilon_0$ [m$^2$/s$^3$]</td>
<td>8381</td>
<td>7888</td>
<td>2074</td>
</tr>
</tbody>
</table>

Table 2

<table>
<thead>
<tr>
<th>Boundary</th>
<th>inlet 1</th>
<th>inlet 2 cold</th>
<th>inlet 2 hot</th>
<th>inlet 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{Z}$ [-]</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$\tilde{T}$ [K]</td>
<td>300</td>
<td>300</td>
<td>1936</td>
<td>300</td>
</tr>
<tr>
<td>$\tilde{u}$ [m/s]</td>
<td>see [9]</td>
<td>0.22</td>
<td>1.5</td>
<td>0.22</td>
</tr>
<tr>
<td>$\tilde{k}$ [m$^2$/s$^2$]</td>
<td>see [9]</td>
<td>$1 \cdot 10^{-5}$</td>
<td>$1 \cdot 10^{-5}$</td>
<td>$1 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$\tilde{\varepsilon}$ [m$^2$/s$^3$]</td>
<td>see [9]</td>
<td>$1 \cdot 10^{-2}$</td>
<td>$1 \cdot 10^{-2}$</td>
<td>$1 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>$\tilde{G}^{\prime \prime}$</td>
<td>$l_F^2$</td>
<td>$l_F^2$</td>
<td>$l_F^2$</td>
<td>$l_F^2$</td>
</tr>
<tr>
<td>$\tilde{\sigma}_t$</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 2

Inlet boundary conditions

The geometry and the boundary conditions used in the simulation are summarized in Fig. 3. Note, that in the experiment a perforated plate is used to generate the pilot flame at inlet 2. Here, the pilot flame and the perforated plate are replaced by an inlet issuing stoichiometric hot burned gas. Table 2 summarizes the inlet boundary conditions for both the cold and hot flow cases. The inlet conditions of the central nozzle for $\tilde{u}$, $\tilde{k}$ are those measured by [9] slightly above the nozzle plane. The inlet profile of $\tilde{\varepsilon}$ for all three flames, reacting and non-reacting, is determined from the only measured distribution of the longitudinal length scale, the cold flow case F2. Outlet boundary conditions are used at the upper and the right boundary, however an inflow of cold ambient air is allowed through the right boundary to account for the entrainment of cold air. The boundaries are sufficiently far away from the flame front so that they do not significantly influence the computed results. Due to the symmetry of the problem, only one half of the experimental setup is
calculated and a symmetry boundary condition is used as the left boundary.

The computational domain of size 145.5 mm x 400 mm in radial by axial direction, is discretized by 119 x 130 non-equidistant grid cells. The smallest grid cells of size 0.5 mm x 1.0 mm are located at the nozzle exit. A numerical flame holder is used to simulate the effect of the pilot flame. It fixes the mean turbulent flame front at the outer edge of the nozzle lip, at $(0 \text{ mm}, 7.5 \text{ mm})^T$.

4.1 Non-Reacting Flow

In order to validate the employed code, figures 4 and 5 show the calculated and measured radial distribution of the axial velocity $\bar{u}/u_0$ respectively turbulent kinetic energy $\bar{k}/k_0$ for the non-reacting case at different downstream locations. Note that no experimental data is available for flame F1, and flame F3 at $x/D_0 = 10.5$ [9] The experimental data shows the spreading of the jet corresponding to the development of two lateral shear layers. After the end of the potential core is reached at approximately $x/D_0 = 4.5$, the maximum mean velocity decreases as the jets expand in the radial direction. The simulation captures these effects well, although the potential core appears to be slightly smaller in the simulation, resulting in marginally earlier spreading of the jet. Also note that employing the proper non-dimensionalization, hardly any difference between the three cases can be discerned, underscoring the self-similarity of all three jets.
The profiles of the turbulent kinetic energy also show the lateral shear layers surrounding the central jet. The turbulent kinetic energy near the centerline increases, indicating the merging of these shear layers and thus the ending of the potential core. Also, the peak turbulent kinetic energy remains nearly constant up to $x/D_0 = 6.5$ for the cases F2 and F3, while it starts to decrease slightly earlier for case F1. Again, hardly any difference can be discerned between all three cases, although case F1 exhibits slightly higher overall values.

Overall, agreement between simulation and experiment for the non-reacting flow is very good.

4.2 Reacting Flow

In this section, results from the RANS level set flamelet model are compared to the experimental data by Chen et al. [9] for the reacting flow case and to the non-reacting flow results presented in the previous section.

Figure 6 shows the radial distribution of the mean temperature $\tilde{T}/T_b$ and the mean axial velocity $\tilde{u}/u_0$ at different axial positions, with $T_b = 2248$ K the adiabatic flame temperature [9]. Compared to the non-reacting case depicted in Fig. 4, the radial profiles of the axial velocity are broadened, meaning that the decreasing slope is shifted to larger radial distances. This is due to the effect of gas expansion in the flame front. As a result, the shear layer is pushed outward in the radial direction. Furthermore, the maximum velocity located at the centerline is almost constant in the axial direction. This indicates, that the potential core is significantly longer than in the non-reacting case. Both these effects are captured well by the simulation and the agreement between simulation and experiment is good.

The measured mean temperature distributions show the trend that the faster the jet exit velocity, the lower the maximum temperature. This can be explained by the fact that the faster the jet exit velocity, the more cold ambient air is entrained on the burned side near the flame, thus reducing the maximum temperature. Also, the higher jet exit velocity flames exhibit a larger flame brush thickness, ie. smaller gradients of the radial temperature distribution. Hence, the adiabatic flame temperature would be reached at larger radial distances, where mixing with the cold ambient air is larger, hence reducing the observed maximum temperature. This effect is reproduced very well by the simulations. The shown decrease in temperature for larger radial distances is due to the mixing with cold ambient air. For flame F3, the maximum temperature initially is overpredicted but is captured very well at $x/D_0 = 8.5$. Also, the simulated flame F3 appears to burn significantly faster in the radial direction than in the experiment, resulting in a significant shift of the
temperature increase to smaller radii. The radial position of the temperature increase, i.e., the flame position is however very well captured for both flames F1 and F2. However, for all three flames, the computed gradient in the ra-
Fig. 5. Radial distribution of turbulent kinetic energy $\tilde{k}/k_0$ for cold cases F1 (left), F2 (center), and F3 (right) at axial positions $x/D_o = 2.5, 4.5, 6.5, 8.5$, and $10.5$. Symbols denote experimental results [9], lines denote numerical results.

dial temperature distribution is larger than in the experiment, indicating that the turbulent flame brush thickness is underpredicted in the simulation. This underprediction is also present in the LES simulations of [27], although to a
Fig. 6. Radial distribution of mean axial velocity $\tilde{u}/u_0$ (●), and mean temperature $\tilde{T}/T_b$ (○) for flames F1 (left), F2 (center), and F3 (right) at axial positions $x/D_o = 2.5, 4.5, 6.5, 8.5$, and $10.5$. Symbols denote experimental results [9], lines denote numerical results.

lesser extend. The reason for this is not directly apparent, however, one potential cause for this behavior is the lack of complete measured turbulent inflow
boundary conditions, specifically the inflow $\tilde{e}$ profile. In [12], only the inlet longitudinal length scale distribution for the cold flow F2 case was measured. This data was used for all three flames both in the non-reacting and in the reacting case. As demonstrated in [13] a change in the turbulent inflow conditions can significantly change the temperature profile of the coherent flame model. No comparison was however presented with the measured turbulent kinetic energy profiles, so that a detailed evaluation of their employed boundary conditions is not possible.

Note also, that the mean temperature at the centerline increases in the experiment for all three flames starting at roughly $x/D_\theta = 4.5$, whereas it stays equal to the unburned temperature in the simulation. This is due to the fact that in the experiment, the instantaneous flame might come close or even cross the centerline resulting in the observed increase in the mean temperature. These larger scale fluctuations are not resolved by the employed RANS approach and are not adequately taken into account in the $G^{\text{th}}$ source terms. Again, this is likely due to the employed inflow boundary conditions. Note that results by Duchamp de Lageneste and Pitsch [27] using a LES turbulence model resolve these instabilities, reproducing the measured axial increase in the mean temperature.

Compared to the RANS results of Prasad and Gore [13] using different flame surface density models, the present results capture the temperature distribution at $x/D_\theta = 2.5$ better. Substantial differences exist in the temperature profiles at $r/D_\theta > 1.2$, where the flame surface density models predict significant more cold air entrainment, such that for $x/D_\theta > 1.4$ the temperature is that of the cold ambient air. The present model, on the other hand predicts significant amounts of hot burned products present at these locations. No experimental data exist for this region to validate either one of these results. At $x/D_\theta = 4.5$ the results of [13] are very similar to those of the present model, however, at $x/D_\theta = 6.5$ the present results show a radially inward shifted flame position that is not present in the coherent flame model analyzed in [13]. At $x/D_\theta = 8.5$, while still capturing the mean flame position well, the coherent flame model underpredicts the maximum temperature, whereas it is well captured by the present model.

Compared to the available LES results by Duchamp de Lageneste and Pitsch [27], the present results are in good agreement at $x/D_\theta = 2.5$, exhibiting the same radial shift of the temperature profile. At $x/D_\theta = 6.5$, however, their shift is less, thus agreeing better with the experimental data.

Figure 7 shows the radial distribution of the turbulent kinetic energy $\tilde{k}/k_0$ at different axial positions. Comparing this to the non-reacting case, Fig. 5, significant differences can be observed. First, the measured maximum values of the turbulent kinetic energy in the reacting case increase for larger axial
Fig. 7. Radial distribution of turbulent kinetic energy $\tilde{k}/k_0$ for flames F1 (left), F2 (center), and F3 (right) at axial positions $x/D_0 = 2.5$, 4.5, 6.5, 8.5, and 10.5. Symbols denote experimental results [9], lines denote numerical results.

distances, whereas they decrease in the non-reacting case. Close to the nozzle the turbulent kinetic energy is thus smaller in the reacting case as compared to the non-reacting case, but far away from the nozzle at $x/D_0 = 10.5$ the reacting
case shows larger values than in the non-reacting case. Second, the location of the maximum value is moving outward with increasing axial distances, not inward as is the case in the non-reacting case. Third, a double maximum in $\tilde{k}$ can be observed in the case of flame F3, with the first maximum located in the unburned gas.

The calculated turbulent kinetic energy distributions differ noticeably from the measured ones. For one, no axial increase in the maximum value of the turbulent kinetic energy is observed, instead an initial decrease followed by an almost constant value from $x/D_o = 4.5$ on is observed. This results in a noticeable underprediction of $\tilde{k}$ further downstream. The reason for this behavior is the fact that the employed $k$-$\varepsilon$ model does not take the effect of gas expansion due to heat release into account. Although the production term in the $\tilde{k}$ equation (14) is proportional to the gradient of the mean velocity, with the gradient being generated by the gas expansion, an increase in the fluctuation of the instantaneous flame front position, i.e. an increase of the turbulent flame brush thickness, decreases the gradient of the mean velocity, thus decreases the production of $\tilde{k}$. In the experiment however, the opposite effect occurs. There, subsequently either burned gas with a large velocity due to gas expansion or unburned gas with a small velocity might be measured at a given point in space. This results in larger values of the RMS velocity, and hence $\tilde{k}$, if the fluctuations of the instantaneous flame front position increases.

Using a LES turbulence model should alleviate the above described problem of the RANS turbulence model, since the mechanism described above should occur to a large extent on the resolved scales of the LES calculation, and hence calculation of $\tilde{k}$ follows the experimental measurement technique described above. Indeed, the LES results by Duchamp de Lageneste and Pitsch [27] capture the increase in turbulent kinetic energy well.

The location of the maximum value of $\tilde{k}$ and hence the outward radial movement of this point is reproduced well by the simulation. Also, the double peak in $\tilde{k}$, with the first maximum located in the unburned gas is well captured by the simulation. This double peak is also present in the F1 and F2 flames, however, the axial position where it first occurs moves downstream the faster the jet exit velocity is. The inner peak than moves toward the centerline where it results in larger simulated values of $\tilde{k}$ than predicted by the experiment. As compared to [6], the results presented here are in slightly better agreement with the experimental data.

Figure 8 shows the shape of the mean turbulent flame front for flames F1 (left), F2 (center), and F3 (right). The numerical result, namely the iso-line $\tilde{G} = G_0$, is denoted by a solid line, whereas the symbols mark the radial position where the measured mean temperature $\tilde{T} = \tilde{T}_{calc}(\tilde{G} = G_0)$. Close to the nozzle at $x/D_o = 2.5$, the measured flames extend radially to the edge of the outer
nozzle wall. Further downstream the flames then burn radially inward. As expected, the higher the nozzle exit velocity, the larger the radial distance of the flame at a given axial distance from the nozzle. Agreement between simulation and experiment is very good for both flames F1 and F2. In the case of flame F3, however, the calculated flame appears to burn significantly faster in the radial direction as compared to the experiment, especially close to the nozzle exit, $x/D_o < 2.5$. There, according to Eq. (24), either $s_L$ or $\tilde{\sigma}_t$ appears to be overpredicted in the simulation.

To analyze this further, Fig. 9 depicts the distribution of the laminar burning velocity made dimensionless with the laminar burning velocity of an unstretched stoichiometric flame $s_L/s_{L, st}$, the mean mixture fraction $\bar{Z}$, its vari-
 ance $\tilde{Z}''$ multiplied by a factor 10, and the mean stretch rate $\tilde{K}$ made dimensionless with the quenching stretch rate $K_q$ along the normalized arclength $s/L$ of the mean flame front, $\tilde{G} = G_0$. Near the nozzle, both flames F1 and F2 exhibit mean stretch rates larger than the quenching stretch rate, hence local extinction occurs, resulting in $s_L = 0$ and hence $s_T = 0$. On the other hand for flame F3, $\tilde{K} < K_q$, thus no quenching occurs and the flame burns inward even close to the nozzle. Also, flame F3 burns in a fully stoichiometric environment ($\tilde{Z} = 1$), whereas flame F2 shows a very small drop in $\tilde{Z}$ to $\tilde{Z} = 0.99$ and F1 shows a drop to $\tilde{Z} = 0.92$. For all three flames, $\tilde{Z}''$ is small, justifying the use of a delta-function PDF for $Z$ in the evaluation of the turbulent burning velocity $s_T$, Eq. (24). Both the mixture fraction distribution but especially the stretch rate distribution result in the laminar burning velocity being largest for F3 and smallest for F1 at any given $s/L$. Compared to the results of [6], the mean flame shapes depicted in Fig. 8, are in significantly better agreement with the experimental data.

Figure 10 shows the radial distribution of some major species’ mass fractions. The entrainment of cold, unburned air is clearly visible in the distribution of $O_2$. Except for the apparent discrepancy in the radial mean flame front position, agreement between simulation and experiment for flame F3 is reasonably good. Absolute values of both CH$_4$ and O$_2$ are well predicted, indicating that the entrainment process of cold ambient air is well captured. Agreement for H$_2$O is good, whereas the levels of CO$_2$ appear to be underpredicted at $x/D_o = 6.5$. Agreement between simulation and experiment for flame F2 is very good. At $x/D_o = 2.5$ the entrainment of cold ambient air seems to be slightly overpredicted resulting in larger values of O$_2$ and smaller values of CO$_2$ and H$_2$O for $r/D_o > 1$. Levels of H$_2$O are very well captured further downstream, while the values for CO$_2$ are consistently slightly underpredicted. The increase of O$_2$ for $x/D_o > 2.5$ and $r/D_o > 0.8$ is very well predicted by the simulation. In the case of flame F1, the amount of entrainment of cold ambient air seems to be overpredicted in the simulation leading to too large levels of O$_2$ for $r/D_o > 0.8$. Levels of CO$_2$ are again consistently underpredicted, as are those for H$_2$O and $x/D_o \leq 6.5$, whereas H$_2$O is captured well for $x/D_o > 6.5$. Overall agreement between experiment and simulation is best for flame F2 and reasonably good for flames F1 and F3.

Figure 11 shows the radial distribution of CO, H$_2$, and OH at different axial positions. In general, the levels of CO are overpredicted by the simulation by a factor of about two. After an initial maximum, CO shows at first a strong decrease followed by a subsequent smaller gradient in the radial distribution for larger values of $x/D_o$. For flame F3, this effect is captured well by the simulation. Levels of H$_2$ are in general underpredicted. The measured distribution shows an inward distinct peak at $x/D_o = 2.5$ that persists up to $x/D_o = 4.5$ for flame F3, $x/D_o = 6.5$ for flame F2, but apparently does not extend beyond $x/D_o = 2.5$ for flame F1. While the simulation results also show a local max-
Fig. 10. Radial distribution of mean CH$_4$ (+,---), O$_2$ (x,- -), CO$_2$ (□,- -), and H$_2$O (■,---) for flames F1 (left), F2 (center), and F3 (right) at axial positions $x/D_0 = 2.5$, 4.5, 6.5, 8.5, and 10.5. Symbols denote experimental results [9], lines denote numerical results.

In H$_2$, the radial location of that maximum is shifted slightly to the outside and does not show the distinct form as is the case in the experiment.
Fig. 11. Radial distribution of mean CO $x10$ ($\circ$, - - -), H$_2$ $x100$ ($\bullet$,------), and OH $x75$ ($\equiv$, - - -) for flames F1 (left), F2 (center), and F3 (right) at axial positions $x/D_\alpha = 2.5$, 4.5, 6.5, 8.5, and 10.5. Symbols denote experimental results [9], lines denote numerical results.

The distribution of OH is generally well reproduced by the computation. Maximum values are well captured, although they are slightly overpredicted for
$x/D_o \geq 4.5$ for flame F3 and $x/D_o \geq 6.5$ for flame F2. While the maximum values close to the nozzle for flame F1 are slightly underpredicted, agreement further downstream is excellent for flame F1. Overall agreement between simulation and experiment is reasonably good. Compared to the results of [6], the mass fraction distributions are significantly improved. This is directly due to the influence of cold ambient air entrainment that was neglected in [6].

To quantify the influence of resolving the instantaneous flame structure as compared to using infinitely fast chemistry, i.e. representing the instantaneous flame as a jump from the unburned to the burned state, Fig. 12 shows a comparison of the radial distribution of OH at three different axial positions for flame F1 calculated with both approaches. Using the resolved flamelets gives clearly superior results as compared to not resolving the inner structure of the instantaneous flame. Using the latter approach underpredicts the measured OH values by a factor of approximately two. It must be pointed out that this result pertains only to mass fraction distributions that exhibit a local maximum in the resolved flame structure. Other distributions, like for example $O_2$ or even the mean temperature $\bar{T}$, show hardly any change at all. Therefore, in order to predict radical levels correctly, the resolved flamelet approach has to be employed, otherwise, the infinitely fast chemistry approach appears to be sufficient.

Figure 13 depicts the calculated distribution of the ratio of flame surface area increase due to turbulence $\tilde{\sigma}_t$ and the flame brush thickness in $G$-space,

$$l_{Ft,G} = \frac{\sqrt{G''}}{|\nabla G'|},$$

made dimensionless by the reference laminar flame thickness $l_{F,ref} = 0.262$ mm. The distribution of $\tilde{\sigma}_t$ for all three flames seems to be very similar. After an initial strong increase close to the nozzle, $\tilde{\sigma}_t$ decreases first with a larger gra-
Fig. 13. Calculated values of $\tilde{\sigma}_t$ (---) and $l_{Ft,G}/l_{Ft,ref}$ (···) along the normalized arclength $s/L$ of the mean flame fronts for flames F1 (left), F2 (center), and F3 (right).

dient, followed by a region of a distinctly lesser gradient. The location of the maximum as well as the point of transition from the larger to the smaller gradient shift downflame with increasing jet exit velocity. The distribution of $l_{Ft,G}$ shows a continuous almost linear increase along the flame, with a distinct change in gradient at the position of the maximum value of $\tilde{\sigma}_t$. It has to be pointed out, however, that $l_{Ft,G}$ is not the turbulent flame brush thickness $\delta_T$,

$$
\delta_T = \left( \frac{\partial \bar{C}'}{\partial r} \right)^{-1} = (T_b - T_u) \left( \frac{\partial \bar{T}}{\partial r} \right)^{-1},
$$

measured in the experiment. Because $\delta_T$ is measured in physical space and $l_{Ft,G}$ relates to $G$ space, it is according to Eq. (34)

$$
l_{Ft} = l_{Ft,G}\tilde{\sigma}_t
$$

that is proportional to $\delta_T$. Figure 14 compares the measured values of $\delta_T$

Fig. 14. Calculated (---) and experimental (···) axial variation of thermal turbulent flame brush thickness $\delta_T$ for flames F1 (left), F2 (center), and F3 (right).

to the ones determined by the simulation. The simulation underpredicts the
measured values by a factor of roughly two. However, the general trend that for flame F3 the flame brush thickness increases and for flame F2 and F1 it stays roughly constant is reproduced by the simulation. For flame F2 a small gradient is still predicted, whereas for flame F1 the calculated values of $\delta_T$ remain roughly constant.

Fig. 15. Production by mean velocity gradients (···), turbulent production (—–), kinematic restoration (— —), and scalar dissipation (– –) of $\bar{\sigma}_t$ along the normalized arclength $s/L$ of the mean flame fronts F1 (left), F2 (center), F3 (right).

Figure 15 shows the relative magnitude of the source and sink terms in the $\bar{\sigma}_t$ equation (26), namely the production by mean gradients, the turbulent production, the kinematic restoration and the scalar dissipation term. The distribution of these four terms is very similar for all three flames and four distinct features can be observed. First, the magnitude of the individual terms increases with increasing jet exit velocity. Second, turbulent production and scalar dissipation clearly dominate both kinematic restoration and production by mean velocity gradients close to the nozzle exit. This indicates that there, all three flames fall well within the thin reaction zones regime. Further downflame, however, both turbulent production and scalar dissipation decrease strongly, so that kinematic restoration cannot be neglected anymore. This indicates that the tip of the flame is considerably closer to the regime of corrugated flamelets than the base of the flame. Third, turbulent production and scalar dissipation exhibit absolute maxima where $\bar{\sigma}_t$ is largest, compare Fig. 13, since they are proportional to $\bar{\sigma}_t$ respectively $\bar{\sigma}_t^3$. Fourth, for flames F1 and F2 kinematic restoration is zero close to the nozzle, because kinematic restoration is proportional to the laminar burning velocity which is quenched in these flames close to the nozzle, compare Fig. 9.

5 Conclusions

We have presented computational results for the three turbulent stoichiometric Bunsen flames F1, F2, and F3 experimentally analyzed by Chen et al. [9]. The results were obtained using the level set flamelet model for premixed
combustion of Peters [1,5], extended to account for the effect of cold ambient air entrainment, coupled to a standard $k-\varepsilon$ turbulence model. The influence of the ambient cold air was taken into account by including a transport equation for the mixture fraction and its variance.

The numerical results have been shown to be in satisfactory agreement with the experimental measurements for flame F3 and in good agreement for flames F1 and F2.

The results show that while a significant amount of cold ambient air is entrained into the outer parts of the flame, the mean flame front still burns either in a purely premixed stoichiometric environment, as is the case for flame F3, or an almost fully premixed stoichiometric environment, as is the case for flames F1 and F2. Premixed combustion models can therefore be directly applied to these flames, however, to capture correctly the composition in the burned gas, it is crucial to take mixing with the entrained cold ambient air into account.

It has been shown that the inner structure of the instantaneous flames has to be taken into account in order to correctly predict mass fraction distributions of species that exhibit a local extremum in their instantaneous mass fraction distribution, for example radicals. Otherwise, the infinitely fast chemistry approach appears to be sufficient to predict all other species distributions, as well as temperature and density fields.

One reason for the observed discrepancies between simulation and measurements is the employed turbulence model in conjunction with the uncertainty in the turbulent inflow boundary conditions. To overcome this problem, the presented level set flamelet model should be coupled to more advanced turbulence models, for example LES. Results for the F2 and F3 flame using a LES turbulence model have been reported in [27] showing improved results. Nevertheless, since RANS turbulence simulations based on $k-\varepsilon$ models are still widely used in industrial applications, the use of these models combined with an advanced turbulent combustion model, i.e. the level set flamelet model, can still yield meaningful results.

**Acknowledgments**

The author would like to express his gratitude to N. Peters, H. Pitsch, and V. Raman for many helpful discussions concerning this work.
References


