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Modeling and Calculation of Turbulent Lifted Diffusion Flames

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Liftoff heights of turbulent diffusion flames have been modeled using the laminar diffusion flamelet concept of Peters and Williams [AIAA J., 21:423–429 (1983)]. The strain rate of the smallest eddies is used as the stretch describing parameter, instead of the more common scalar dissipation rate. The $h(U)$ curve, which is the mean liftoff height as a function of fuel exit velocity can be accurately predicted, while this was impossible with the scalar dissipation rate. Liftoff calculations performed in the flames as well as in the equivalent isothermal jets, using a standard $k-\varepsilon$ turbulence model yield approximately the same correct slope for the $h(U)$ curve while the offset has to be reproduced by choosing an appropriate coefficient in the strain rate model. For the flame calculations a model for the pdf of the fluctuating flame base is proposed. The results are insensitive to its width. The temperature field is qualitatively different from the field calculated by Bradley et al. (Twenty-Third Symposium on Combustion, 1990, pp. 685–692) who used a premixed flamelet model for diffusion flames.

INTRODUCTION

Turbulent jet diffusion flames constitute an important class of flames, in theoretical and experimental studies as well as in industrial applications, such as gas turbine combustors and flare burners.

For most fuels liftoff of the flame occurs at fairly low fuel exit velocities, and consequently liftoff is an important phenomenon. A lifted turbulent diffusion flame consists of a cold flow near field region and a nonequilibrium flame region, separated by the fluctuating flame base. The distance from the nozzle to the flame base is called the liftoff height. The physical mechanism that is responsible for the lifting of the flame is the competition between flow and chemical effects, characterized by their respective time scales, the ratio of which is the Damköhler number. If typical chemical time scales are everywhere smaller than flow residence times, the flame will be rim stabilized. If the fuel exit velocity increases, then the residence time, which is the inverse of a strain rate, decreases and so does the Damköhler number. At a critical exit velocity the flame can no longer be stable at the nozzle rim and liftoff occurs. From this point increasing the fuel velocity further leads to an increase of the liftoff height proportional to the exit velocity [1]. This regime is the subject of the present paper.

Current prediction methods for rim stabilized turbulent diffusion flames are reasonably accurate [2, 3]. For flames with liftoff the main difficulty is the accurate prediction of the liftoff height for which there exist two major classical proposals. The oldest considers the base of the flame as a premixture of fuel and oxidizer. The burning velocity of this mixture equals the flow velocity at the flame base [4]. Peters and Williams [5], however, have argued that no sufficient premixing of the reactants can take place for this concept to be valid, in accordance with experimental results of Pitts [6]. Therefore they proposed a liftoff theory based on laminar diffusion flamelet quenching. Laminar counterflowing diffusion flames, called flamelets, are extinguished if the stretch experienced by the flame exceeds a critical quenching value [7]. If a turbulent diffusion flame may be considered as an ensemble of laminar diffusion flamelets with all different stretch rates [8], then liftoff of a turbulent flame can be described with this concept [5]. The liftoff condition is obtained by realizing that liftoff is a threshold phenomenon. The variable that is responsible for this behavior is the fraction of...
burnable flamelets, or the probability of burning [5]. The probability of burning is defined in terms of a variable describing stretch effects, and usually the scalar dissipation rate is chosen for this purpose [5]. If this quantity is used in the liftoff condition, predicted liftoff heights are not in very good agreement with experiments.

A third concept for predicting liftoff heights of turbulent diffusion flames was proposed by Bradley et al. [9] with an alternative, so called mixedness-reactedness, flamelet model. Here the combustion is considered to take place in a premixed mode in the diffusion flame. At each given mixture fraction within the flammability limits, a premixed flame is established. Because the most obvious independent parameter for a premixed flame is the temperature, instead of the mixture fraction, all scalar profiles are given in terms of the temperature. In this way, the heat release in temperature space is determined, and the mean heat release is calculated by integrating over independently chosen probability density functions for mixture fraction and temperature. The liftoff height is determined by the axial distance where the mean heat release begins. The obtained liftoff heights as a function of fuel exit velocity \( h(U) \) correspond well with the experimental data of Kalghatgi [1]. Despite the success of this method, it is not completely clear whether the assumption of premixing is justified. Furthermore apparently no threshold behavior is contained in the model, while this is a very characteristic feature of a lifting flame.

Therefore in the present article attention will be focused on the liftoff mechanism based on laminar diffusion flamelet quenching of Peters and Williams [5, 10] mentioned earlier. Predictions of the liftoff height based on this concept have been made by considering the equivalent isothermal jet flow [5, 11], but the slopes of the \( h(U) \) curves were not in agreement with experiments.

Very recently Peters [12] modeled the liftoff height using the strain rate of the large eddies instead of the scalar dissipation rate in the liftoff condition. The calculated liftoff heights, based on isothermal jets are in good agreement with experiments.

In the present work the liftoff height will be predicted based on the flow fields of the isothermal jet as well as of the flame. The strain rate will be used in the liftoff condition instead of the scalar dissipation rate. The reasons for choosing this variable are discussed. In the flame calculations a probability density function (pdf) for the liftoff height, which takes care of the fluctuating flame base, is proposed and the influence of the shape of this function on the predicted temperature profiles is investigated. The influence of variable density effects on the predicted liftoff height is determined by comparing predicted liftoff heights in the flame with liftoff heights obtained from isothermal jet calculations.

**ANALYSIS**

Two main problems characterize the calculation of a lifted turbulent diffusion flame. Firstly the mean liftoff height has to be determined. Secondly the fluctuating behavior of the flame base must be taken into account.

**Modeling of the Liftoff Height**

If lift off occurs through laminar diffusion flamelet quenching, then the topology of the lifted flame is a disconnected surface of instantaneous stoichiometry. By the disconnectedness local quenching of the flame is meant. This is caused by local values of the stretch or nonequilibrium parameter, higher than the quenching value. At these points no flame can exist, and these positions are called holes [10]. The fraction of burnable flamelets, which is equal to one minus the probability that a hole is present at a certain position, can be estimated by integrating the pdf of the relevant stretch parameter up to the quenching value of a laminar diffusion flame. This fraction of burnable flamelets is also called the probability of burning

\[
P_b = \int_0^{\Omega_q} P(\Omega) \, d\Omega,
\]

in which \( \Omega \) is the stretch parameter, which can be the scalar dissipation rate \( \chi \) as in refs. 5 and 11 or the strain rate \( s \). The quenching value \( \Omega_q \) is determined from laminar diffusion.
flamelet calculations [13–15] or from experiments [10]. The form of the pdfs $P(\Omega)$ are a lognormal distribution for the scalar dissipation [5] and a quasi Gaussian pdf for the strain rate [16]. The latter is written as

$$
P(s) = \frac{2}{(2\pi\sigma_s)^{1/2}} \exp\left(-\frac{s^2}{2\sigma_s^2}\right).
$$

Here $\sigma_s$ denotes the variance. The mean and variance are coupled by

$$
\tilde{s} = \left(\frac{2}{\pi}\right)^{1/2} \sigma_s.
$$

If too many holes are present, or the probability of burning is too low, on the contour of stoichiometric mixture where the flame is located instantaneously, the flame cannot be stabilized at the burner rim and liftoff occurs. The fraction of holes which is allowed until the flame lifts off can be roughly estimated with percolation theory. This theory can be used to describe the threshold behavior of the liftoff of the flame by means of the probability of burning [10]. This concept leads to a liftoff condition involving both a percolation threshold $P_c$ and a probability of burning $P_b$ [5]

$$
P_b = P_c
$$

at a radial position where the mean mixture fraction $\tilde{f}$ is stoichiometric $\tilde{f} = f_{st}$. If Eq. 4 is used at the mentioned radial position, with the appropriate pdf $P(\Omega)$ inserted into Eq. 1 for $P_b$, then a relationship is obtained between $\Omega_q$ and the mean $\bar{\Omega}$, with the variance of $\Omega$ as a parameter. The mean and variance of $\Omega$ are supposed to completely determine the pdf $P(\Omega)$. The above procedure leads to the following liftoff condition if the strain rate is used for $\Omega$

$$
P_c = \text{erf}\left(\frac{s_q}{\tilde{s}(r = r_{st})\pi^{1/2}}\right),
$$

where $r$ is the radial distance from the symmetry axis. If the value of $P_c$ is about 0.63 [5], then this equation can be simplified to approximately

$$
\tilde{s}(r = r_{st}) = \frac{s_q}{P_c \pi^{1/2}}.
$$

If the scalar dissipation rate is used, then the simple liftoff condition

$$
\tilde{s}(r = r_{st}) \approx \sigma_q
$$

is obtained with $P_c = 0.63$ and $\sigma_q = 0.5$ [5].

In the following several arguments are given to support the choice of the strain rate for $\Omega$, and the practical justification of this choice will be given by the results of this article in which the slope of the $h(U)$ curve is the main important parameter.

Four arguments are presented in favor of the strain rate as the stretch parameter.

Firstly laminar counterflow diffusion flames are considered. They are the cornerstone for laminar flamelet models in turbulent combustion [8]. In these counterflow diffusion flames the strain rate imposed on the flame gives rise to stretch effects, leading to nonequilibrium chemistry. The scalar dissipation rate is just the consequence of this strain rate. Additionally, the scalar dissipation rate is zero at both cold flow boundaries, which necessitates the introduction of a particular location in the flame, where the scalar dissipation rate should be evaluated. Often the scalar dissipation rate at stoichiometric conditions $X_{st}$ is chosen [8], but conditioning of the scalar dissipation rate on a specific value of the mixture fraction leads to a fundamental problem. The flamelet concept leads to the following general expression for the mean of a scalar

$$
\Phi = \int_0^1 df \int_0^{\infty} d\Omega P(f, \Omega) \phi(f, \Omega),
$$

in which $P(f, \Omega)$ is the joint probability density function for the mixture fraction and the stretch parameter $\Omega$ and $\phi(f, \Omega)$ is a scalar and a function of the mixture fraction with $\Omega$ as a parameter. If $\Omega$ is chosen to be the scalar dissipation rate conditioned on stoichiometry ($\Omega = \chi(f = f_{st})$) then $P(f, \chi_{st})$ has no meaning other than $P(\chi_{st})$. This is not realistic because no account would be taken of the mixture fraction fluctuations. In practical calculations this inconsistency has been solved by simply stating that there is no satisfactory
model for the conditioned scalar dissipation rate, and so the unconditioned model \( \bar{\chi} = 2\bar{\varepsilon}/\bar{k} \) was used, with \( \bar{\varepsilon} \) the scalar variance and \( \bar{k} \) the turbulent kinetic energy. In that case, assuming statistical independence, \( P(f, \Omega) = P(f)P(\Omega) \), the integral in Eq. 8 can be done. The strain rate, however, need not be conditioned on any particular mixture fraction value because it is a boundary condition in a counterflow diffusion flamelet, so this problem does not arise.

Secondly a more serious problem is the increase of the quenching value of the scalar dissipation rate at quenching of a laminar counterflow diffusion flamelet if the fuel mass-fraction at the fuel boundary is decreased. This is contrary to the value of the strain rate at quenching, which decreases with decreasing fuel mass-fraction, as it should. These observations can be inferred from Fig. 10 in Ref. 8, and from flamelet calculations performed in the present work (see Fig. 1), where the calculated quench values \( a_q \) and \( \chi_q \) are plotted versus the methane volume fraction in diluted methane–air counterflow diffusion flames. Consequently, if the scalar dissipation rate is used as the stretch parameter, then the application of the liftoff condition as described above, would yield shorter liftoff heights if the fuel stream is diluted, which is unphysical. The experiments of Miake-Lye and Hammer [17] indeed indicate an increase of the liftoff height if the fuel is diluted, even though air was used for dilution instead of an inert gas.

Thirdly, in both Refs. 5 and 11 a liftoff condition similar to Eq. 7 was used. The slopes of the predicted \( h(U) \) curves were not in agreement with the experiments. The discrepancies might be explained by the different scaling properties of the scalar dissipation rate and the strain rate. The scalar dissipation rate on the axis of an isothermal axisymmetric jet scales with \( x^{-4} \) while the strain rate scales with \( x^{-2} \). Although the points where the mean mixture fraction is stoichiometric are not located on the axis, it is fair to say that there is a large difference between these two variables regarding their scaling properties. Due to the slower decrease of the strain rate in axial direction, the liftoff condition, Eq. 6 will be met at higher \( x \)-values leading generally to higher liftoff heights in better agreement with experiments.

Lastly, if the scalar dissipation rate is retained as the descriptor of stretch effects, it still essentially is a strain rate [18]. This is due to the fact that the flame thickness in mixture fraction space is constant, independent of the stretch imposed on the flamelet. Eventually the scalar variance \( \bar{\varepsilon} \) is replaced by the flame thickness, leading to a scalar dissipation rate at the position of the flame \( \chi_f \sim \bar{\varepsilon}/\bar{k} \), which essentially is the strain rate of the large eddies. The details of this analysis are given by Peters [12].

**Modeling of the Fluctuating Flame Base**

The fluctuating flame base will be handled by introducing a pdf for the location of the flame base \( P(x_f) \) where \( x_f \) denotes the axial distance from the nozzle to the flame base. The mean scalar quantities such as density and temperature can now be written as

\[
\overline{\phi}(x) = \int_0^x P(x > x_L) dx_L \int_0^1 df \times \int_0^\infty ds P(f, s) \phi(f, s) + \left(1 - \int_0^x P(x > x_L) dx_L \right) \int_0^1 P(f) \phi(f) df.
\]

In this equation the last term is the isothermal
value of the scalar, and the factor in front of it is the probability that the flame base is located downstream of $x$. The probability that the instantaneous flame base is upstream of $x$ is denoted by $P(x > x_L)$. The first term in Eq. 9 is valid in the burning part of the jet, and is due to both burning and nonburning flamelets, where the average must be calculated over the mixture fraction and the strain rate and their appropriate pdfs. Statistical independence between the mixture fraction and strain rate must be assumed if no transport equations for pdfs are solved, so $P(f, s) = P(f)P(s)$. In this work presumed shapes for $P(f)$ and $P(s)$ are taken, namely a beta function for the first and a quasi-Gaussian for the latter. The pdf for the flame base is unknown. To calculate it, two point pdfs are needed, which is computationally intractable for this situation. Therefore a proposition for this pdf is made. The form is assumed to be a triangle pdf around the mean liftoff height $h$ determined from the liftoff condition, and the width is taken to be 5 diameters.

**TURBULENCE AND COMBUSTION MODELING**

**Turbulence Model**

The turbulent reacting flow is modeled using Favre-averaged quantities [19-21] together with the $k-\varepsilon$ turbulence model. The Favre-averaged velocity vector is denoted by $\bar{U}$ and its Favre fluctuation by $\tilde{u}$. The Favre-averaged turbulent kinetic energy, its dissipation rate, the mixture fraction fluctuations and the scalar dissipation rate are denoted by $\bar{k}$, $\tilde{\varepsilon}$, $\tilde{f}$, and $\tilde{\chi}$, respectively. The pressure and density are conventionally time averaged and denoted by $\bar{p}$ and $\bar{\rho}$, respectively.

The equations consist of the continuity equation

$$\nabla \cdot (\bar{\rho} \bar{U}) = 0$$  \hspace{1cm} (10)

and the momentum equation

$$\nabla \cdot (\bar{\rho} \tilde{U} \bar{U}) = -\nabla \bar{p} + \nabla \cdot \tau.$$  \hspace{1cm} (11)

No buoyancy terms are included because the flame under consideration is completely momentum driven in the region of interest. The Reynolds stress tensor is modeled as

$$\tau_{ij} = -\bar{\rho} \tilde{u}_i \tilde{u}_j = -\frac{2}{3} \delta_{ij} \left( \bar{\rho} \bar{k} + \mu \nabla \cdot \tilde{U} \right)$$

$$+ \mu \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right),$$  \hspace{1cm} (12)

where $\delta_{ij}$ is the Kronecker delta. The turbulent viscosity is modeled as $\mu_t = C_{\mu} \bar{\rho} \bar{k}^2 / \tilde{\varepsilon}$.

The turbulence model consists of equations for the turbulent kinetic energy $\bar{k}$ and dissipation $\tilde{\varepsilon}$. The kinetic energy equation is

$$\nabla \cdot (\bar{\rho} \bar{k} \tilde{U}) = \nabla \cdot \left( \frac{\mu_k}{\sigma_k} \nabla \tilde{k} \right) + P_k - \bar{\rho} \bar{\varepsilon},$$  \hspace{1cm} (13)

with $P_k$ the production term of turbulent energy $-\bar{\rho} \tilde{u}_i \tilde{u}_j \frac{\partial \bar{U}_i}{\partial x_j}$. The dissipation equation is

$$\nabla \cdot (\bar{\rho} \tilde{\varepsilon} \tilde{U}) = \nabla \cdot \left( \frac{\mu_\varepsilon}{\sigma_\varepsilon} \nabla \tilde{\varepsilon} \right) + \frac{\tilde{\varepsilon}}{k} (C_1 P_k - C_2 \bar{\rho} \bar{\varepsilon}).$$  \hspace{1cm} (14)

Furthermore the equations for the mixture fraction $\tilde{f}$ and scalar variance $\tilde{\chi} = f_\text{mix}^2$ are

$$\nabla \cdot (\bar{\rho} \tilde{f} \tilde{U} \tilde{U}) = \nabla \cdot \left( \frac{\mu_f}{\sigma_f} \nabla \tilde{f} \right),$$  \hspace{1cm} (15)

$$\nabla \cdot (\bar{\rho} \tilde{\chi} \tilde{U}) = \nabla \cdot \left( \frac{\mu_\chi}{\sigma_\chi} \nabla \tilde{\chi} \right) + P_\chi - \bar{\rho} \tilde{\chi}.$$  \hspace{1cm} (16)

Here $P_\chi$ is the production term of scalar fluctuations $-\bar{\rho} \tilde{u}_i \tilde{u}_j \frac{\partial \tilde{f}}{\partial x_i}$. The scalar dissipation rate $\tilde{\chi}$ is modeled according to standard practice by assuming equality of velocity and scalar integral length scales: $\tilde{\chi} = C_{\chi,1} \bar{\rho} \bar{\varepsilon} / \bar{k}$, where the coefficient $C_{\chi,1}$ is empirical and usually taken to be equal to 2. The assumption of equal length scales leads to fixed turbulent
Schmidt numbers $\sigma_f$ and $\sigma_g$ in the scalar transport model.

$$-\bar{p}u_i\bar{f} = \frac{\mu_i}{\sigma_f} \frac{\partial \bar{f}}{\partial x_i}. \quad (17)$$

The constants in above equations are given in Table 1. A scalar transport model that does not assume equal length scales and fixed turbulent Schmidt numbers is given by Sanders and Lamers [22]. The expression for the scalar dissipation rate obtained with this model is

$$\tilde{\chi} = C_{x,2} \tilde{g}^{\lambda_1} \tilde{\varepsilon}^{\lambda_2}, \quad (18)$$

with $\lambda_1 = 1.5$ and $\lambda_2 = 0.25$ determined from isothermal jet calculations and $C_{x,2}$ a coefficient (not dimensionless) to be adjusted to experimental data.

To be able to use the liftoff condition (Eq. 6) the strain rate must be modeled. If the strain rate $s$ is interpreted to be the strain rate of the smallest eddies then

$$\tilde{s} = C_{s,1} \left( \frac{\tilde{\varepsilon}}{2 \nu} \right)^{1/2} \quad (19)$$

which is based on the concept of dissipation of turbulent energy by strain rate fluctuations on the smallest scales. This explains the molecular viscosity $\nu$ in Eq. 19. The coefficient $C_{s,1}$ in this equation is unknown, but it will be determined in the course of the work. If $s$ is interpreted as the strain rate of the large eddies, then

$$\tilde{s} = C_{s,2} \frac{\tilde{\varepsilon}}{k}, \quad (20)$$

and also here, the coefficient $C_{s,2}$ has to be determined later on.

A short discussion on the scaling properties of both strain rates with axial distance and fuel exit velocity is in order because both strain rates vary as $x^{-2}$ on the axis of an axisymmetric jet that might give the impression that they are completely similar. In the first place it must be mentioned that the strain rates are used in the liftoff condition only along the line of stoichiometric mixture, which makes an asymptotic scaling analysis somewhat difficult to perform since this line of stoichiometric mixture forms a closed contour and consequently does not exist at very large $x$. Nevertheless different scaling properties on the axis will also have their influence on the line of stoichiometric mixture.

The axial scaling properties of $\tilde{\varepsilon}$, $\tilde{k}$, and $\tilde{U}_f$ are: $\tilde{\varepsilon} \sim \tilde{U}_f^{3/2} x^{-1}$, $\tilde{k} \sim \tilde{U}_f^2$ and $\tilde{U}_f \sim \tilde{U} x^{-1}$. Inserting these expressions into the equations for the strain rates gives a scaling behavior of $\tilde{s} \sim \tilde{U}_f^{3/2} \nu^{-1/2} x^{-2}$ for the small eddy strain rate and $\tilde{s} \sim \tilde{U} x^{-2}$ for the large eddy strain rate. Consequently both strain rates have the same $x$-scaling behavior but scale differently regarding $\tilde{U}$. Additionally it may be remarked that along the line of stoichiometric mixture both strain rates vary approximately as $x^{-1}$, although at small $x$ the large eddy strain rate falls off more rapidly.

**Combustion Model**

Combustion is modeled by introducing the combustion invariant mixture fraction $f$ [23], which is only convected and diffused through the flow. Considering the mixture fraction as an independent variable, all scalars except the pressure are coupled to the mixture fraction by invoking the flamelet concept [8, 24]. Each flamelet is characterized by the value of the strain rate experienced by the flamelet. So at each strain rate a table of scalars versus mixture fraction exists. The total of tables is called a flamelet library. In the present work main attention is focused on fluid mechanical processes in the lifted flame. From numerical calculations and from literature it is known that a flamelet library consisting of two flamelets, one burning and the other isothermal, is accurate enough for purposes of determining the mean density and temperature. Consequently the
integral in Eq. 9 can be written as follows

\[ \tilde{\phi}(x) = P_d P_b \int_0^{1} \tilde{P}(f) \phi_b(f) \, df \]
\[ + ((1 - P_b) P_d + P_u) \times \int_0^{1} \tilde{P}(f) \phi_o(f) \, df. \]  

(21)

In this equation, \( P_b \) is given by Eq. 1 with the appropriate pdf, the subscript \( b \) denotes the burning flamelet, and the subscript \( o \) denotes the isothermal value. \( P_a \) is the abbreviation for \( \int_0^{x_L} P(x > x_L) \, dx_L \), the probability that the location \( x \) is downstream of the mean lift off position and \( P_u \) is the complementary probability. The beta function pdf for the mixture fraction has the form

\[ \tilde{P}(f) = f^{a-1}(1 - f)^{b-1}/\beta(a, b) \]  

(22)

with \( a = \bar{f}(\bar{f}(1 - \bar{f})/\bar{g} - 1) \) and \( b = a(1 - \bar{f})/\bar{g} \)

\[ \beta(a, b) = \int_0^{1} f^{a-1}(1 - f)^{b-1} \, df \]  

(23)

In the flow calculations, the conventional time averages for the density and temperature are needed, and therefore for these variables, Eq. 21 is rewritten as [25]

\[ \bar{\rho}(x) = \frac{P_d P_b}{\int_0^{1} \tilde{P}(f)/\rho_b(f) \, df} \]
\[ + \frac{(1 - P_b) P_d + P_u}{\int_0^{1} \tilde{P}(f)/\rho_o(f) \, df}. \]  

(24)

and

\[ \bar{T}(x) = \frac{P_d P_b}{\bar{\rho}_b \int_0^{1} \tilde{P}(f) T_b(f)/\rho_b(f) \, df} \]
\[ + \frac{(1 - P_b) P_d + P_u}{\bar{\rho}_o \int_0^{1} \tilde{P}(f) T_o(f)/\rho_o(f) \, df}. \]  

(25)

COMPUTATIONAL SETUP

Turbulent Flow Calculations

The experimental results used to compare with the numerical predictions are those of the free vertical natural gas jets and lifted flames measured by Wittmer [26]. The fuel exit velocities in the jet and flame are between 40 and 71 m/s with a slow coflowing air stream of 0.4 m/s. The nozzle diameter \( D \) is 8 mm.

Due to the fluctuations of the flame base, there might be a back coupling from downstream to upstream positions in the flame [9]. This necessitates the use of an elliptical computer code. The finite volume computer code Teach [27] was chosen as a framework for this study.

Most calculations were performed on a rectangular grid consisting of \( 80 \times 50 \) nodes in axial and radial direction, respectively.

Boundary Conditions

Variables at the radial boundary are zero, except the axial velocity, which is equal to the free stream velocity, and the radial velocity that was determined by the continuity equation. At the outlet zero gradients are applied. At the inlet a flat velocity profile was imposed and the turbulent kinetic energy was taken as \( \bar{k} = U^2/1000 \) and the dissipation as \( \bar{\varepsilon} = C_u \bar{k}^{3/2}/0.03D \). The mixture fraction at the inlet is equal to 1 and its fluctuation is 0.

Flamelet Calculations

Prior to solving the elliptical equations given in the previous section, the scalar profiles as a function of mixture fraction with the strain rate as a parameter in a laminar counterflowing diffusion flame are needed. These profiles are obtained by numerical integration of the boundary layer similarity equations describing two counterflowing streams [28]. The equations solved are the continuity, momentum, temperature, and species equations. The numerical code essentially is a damped and modified Newton method [29]. This flamelet code is only used as a tool and not described in this article. The program is a precursor of the Cambridge flamelet code RUNIDL [30].

The profiles that are used in the present work are the density and temperature as a function of mixture fraction.
RESULTS

Isothermal Jets

The isothermal flow is used to get an indication of the usefulness of the several liftoff models. The upstream part of the flow in a lifted flame is mainly isothermal, but in the vicinity of the flame base variations in temperature and density are steep. Therefore the isothermal flow is only a first approximation. To get an idea of the accuracy of the calculations in the isothermal flow, the curve of radial position where the mean mixture fraction is stoichiometric as a function of axial distance is compared with measurements of Horch \[31\] (Fig. 2).

The agreement between measurements and calculations is very good for \(x/D < 20\). The deviation of 13\% farther downstream could be caused by both an experimental uncertainty and a model deficiency.

Liftoff heights are calculated with four different liftoff conditions. The first and second are based on two different modeling assumptions for the strain rate, see Eqs. 19 and 20, while the third and fourth are based on the scalar dissipation rate as the relevant stretch parameter. For liftoff calculations alone, the scalar dissipation rate was modeled according to \(\dot{\chi} = C_{\chi,1} \bar{\varepsilon} g / k\) and \(\dot{\chi} = C_{\chi,2} \bar{\varepsilon}^{1.5} e^{0.25}\). Although the strain rate already was chosen to be the appropriate stretch parameter, the results obtained with the scalar dissipation rate serve as an indication for the superior of using the strain rate.

The quenching values for the strain rate and scalar dissipation rate are \(s_q = 565 \text{ s}^{-1}\) and \(\chi_q = 48 \text{ s}^{-1}\), which are obtained from laminar diffusion flamelet calculations of a planar flamelet.

The coefficients \(C_{s,1}\) and \(C_{s,2}\) in the strain rate models and the coefficient \(C_{\chi,1}\) and \(C_{\chi,2}\) in the scalar dissipation model are to be determined. To this end the liftoff height of the flame with exit velocity of 71 m/s is taken as a reference. The coefficients are adapted so as to reproduce this liftoff height. Using the obtained value in the cases with the lower exit velocities as well, the \(h(U)\) curve given in Fig. 3 is obtained.

It must be noted that in the turbulent flow equation for the mixture fraction fluctuations \(\bar{\varepsilon}\) the standard model \(\dot{\chi} = C_{\chi,1} \bar{\varepsilon} g / k\) with \(C_{\chi,1} = 2\) was used and only in the lift off condition the coefficients \(C_{\chi,1}\) and \(C_{\chi,2}\) are adapted.

It is clearly seen in Fig. 3 that the curve with the strain rate of the smallest eddies with \(C_{\chi,1} = 0.116\) gives the best results. The curve obtained if the strain rate of the large eddies is used with \(C_{\chi,2} = 6.4\) is also satisfactory.

In order to give an indication of the sensitivity of the \(h(U)\) curve with respect to, for instance, \(\nu\) or \(C_{s,1}\), the viscosity has been varied by factors of 2. As this is equivalent to varying \(C_{s,1}\) at constant \(\nu\), a vertical shift of the \(h(U)\) curve is to be expected. A lower strain rate (higher \(\nu\)) will shift the curve downwards, while a higher strain rate will shift it upwards. This is illustrated in Fig. 4, where it is also observed that the slope of the curves is hardly influenced, which indicates that it is determined mainly by the dynamics of the stretch describing parameter.

The liftoff heights obtained with the scalar dissipation rate with \(C_{\chi,1} = 423\) do not agree with the experimental results. Furthermore this large value of \(C_{\chi,1}\) is at variance with the normally accepted value of \(C_{\chi,1} = 2\). The reason for this unacceptable discrepancy is the fact that in this work the coefficient is adapted, so as to reproduce the experimental liftoff height at a fuel exit velocity of 71 m/s. If the standard model of the scalar dissipation rate with \(C_{\chi,1} = 2\) was used the liftoff heights would
be very severely underpredicted. The slope of the \( h(U) \) curve obtained with the second model for the scalar dissipation rate, with \( C_{x,2} = 1.8 \times 10^5 \) is underpredicted as well. Also in this case the value of \( C_{x,2} \) is much larger than the value which was used in a previous study [22], namely \( C_{x,2} \approx 730 \). However, even with the higher values for \( C_{x,1} \) and \( C_{x,2} \) the slopes of the curves are underpredicted. An underpredicted slope was also found by Peters and Williams [5] (Fig. 5), who used the liftoff data of Horch [31] of a natural gas jet flame. This indicates that the scalar dissipation rate is not the correct variable to use.

The fact that the liftoff heights in Fig. 5 are not severely underpredicted is partly due to the lower quenching value of the scalar dissipation, namely \( X_q = 5 \) s\(^{-1}\), instead of the current \( X_q = 48 \) s\(^{-1}\). There is significant uncertainty about the exact value of \( X_q \), and because this value mainly determines the base of the \( h(U) \) curve, most attention should be paid to the slope of the curve, and this is predicted well with the strain rate of the smallest eddies.

From the above it may be concluded that the strain rate of the small eddies is the relevant stretch parameter. However, because these calculations correspond to an isothermal flow without strong density variations the first model of the strain rate will be tested in a real flame.

**Lifted Flames**

The flame calculations are performed with the liftoff condition described by Eqs. 6 and 19. The pdf of the liftoff height is used to calculate the scalar variables such as density and temperature, according to Eq. 9. The form of this pdf is chosen to be a triangle with a width of 5 diameters. This value is taken from Ref. 32, but its exact value only marginally influences the calculations.

The combustion is modeled using the flamelet concept, with two flamelets. One is burning and experiences a strain rate of 100 s\(^{-1}\) and the other is isothermal.
In Fig. 6 the liftoff height as a function of exit velocity is given. The calculations correspond extremely well with the experiments. However, the coefficient $C_{s,1} = 0.27$ is larger than in the isothermal jet calculations. This is due to the increase of molecular viscosity with temperature. Thereby the strain rate in Eq. 19 evaluated at $\dot{f} = f_{st}$ decreases sharply in the flame zone. To match the liftoff condition, the coefficient $C_{s,1}$ has to be increased. This coefficient mainly determines the actual liftoff height but does not influence the slope of the curve and therefore this most important feature of the flame can be accurately predicted both with isothermal and non isothermal calculations.

It is noticeable that Bradley et al. [9] with their mixedness-reactedness flamelet model used a value for $C_{s,1}$ of the same order of magnitude, namely $C_{s,1} = 0.081$. Given the fact that there is no universally accepted value for this modeling constant and that Bradley et al. [9] used a different flamelet model, this correspondence is remarkable.

The predictions of the axial velocity in the flame are given in Fig. 7. The sudden onset of combustion, accompanied by the temperature rise, leads to an expansion effect that generates the spike in the calculated velocity profile. This is not measured, but possibly the axial distances between the measuring stations are too large to allow a detection of this sort. The expansion-induced difference between the isothermal and flame calculation is visible downstream of the mean liftoff height.

The temperature contours in the flame with exit velocity 71 m/s are presented in Fig. 8. It can be seen that the contours of maximum temperature show behavior, for instance the hollow center of the flame base [17, 33], which is to be expected in a lifted flame. This figure can be compared with Fig. 4 given in Ref. 9. The main difference is the axial position where the mean temperature starts to increase on the symmetry axis. In Fig. 8 this position is approximately equal to the mean liftoff height while in Fig. 4 in Ref. 9 this position is roughly 4 times the liftoff height. Because there are no experiments available, it is difficult to make a judgment about this discrepancy. However, due to strong turbulence mixing, it seems likely that heat generated at the mean flame position diffuses towards the axis more rapidly, such as in Fig. 8. On the other hand, if a velocity spike such as present in Fig. 7 is not in agreement with experiments, a less strong temperature rise on the symmetry axis is to be expected, which could be in favor of the results presented in Ref. 9.

CONCLUSIONS AND DISCUSSION

Turbulent lifted natural gas diffusion flames have successfully been modeled and calculated using a $k-\varepsilon$ turbulence model and the laminar diffusion flamelet concept. The most difficult aspect of the flame, namely the liftoff height, has been calculated in the flame as well as in the equivalent isothermal jet. From these cal-
calculations it can be inferred that the strain rate instead of the scalar dissipation rate is the relevant parameter to describe stretch effects in turbulent flames. The resulting curves of the liftoff height as a function of fuel exit velocity \( h(U) \) are in good agreement with experiment if the strain rate of the smallest eddies is used, while the strain rate of the large eddies gives satisfactory results. The correct slope in both the isothermal jet as well as in the flame is obtained, while the only coefficient in the model for the strain rate that has to be fitted fixes the absolute liftoff height at one fuel exit velocity. This coefficient has no generally accepted value. In this study it also serves to take account of possible uncertainties in the numerical values of \( s_0 \) and of the percolation threshold \( P_c \). Its value is about 2 times larger in the flame than in the isothermal case, which is due to temperature and density effects in the flame. The close agreement between isothermal and flame based \( h(U) \) curves, supports the conclusion of Pitts [34] that isothermal mixing processes can be used to describe flame stabilization mechanisms.

The calculation of the turbulent flame comprises a model for the fluctuating flame base. The scalar variables, such as density and temperature, are calculated using a probability density function for the liftoff height. The exact form of this pdf being unknown a triangle pdf is proposed. Numerical variations of the width of this pdf showed no significant influence on the results.

The axial velocity profile in the flame exhibits a spike as a consequence of expansion effects in the vicinity of the liftoff position. Experimental data do not show this spike, but it is unknown whether it is just not resolved, or is a flaw in the proposed model for the fluctuating flame base.

Calculated temperature profiles show an earlier increase of the temperature on the symmetry axis than do the temperature profiles of Bradley et al. [9], obtained with a flamelet model based on premixed combustion. No judgment can be made because no temperature measurements are available.

The major conclusion of this work is that it is possible to accurately calculate the liftoff height of a turbulent diffusion flame with the laminar diffusion flamelet concept if the strain rate instead of the normally used scalar dissipation rate is used. Furthermore, isothermal jet calculations do allow a correct slope of the \( h(U) \) curve to be determined, but the coefficient in the strain rate then has a slightly different value compared with the one in the flame.

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REFERENCES

on laminar and turbulent combustion, Aachen, 1992, pp. 156–166.

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