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The numerical analysis of a diffusion flame in a reacting, two-dimensional, turbulent, viscous, multicomponent, compressible mixing layer subject to an axial pressure gradient is presented. The boundary layer equations for the mean values of axial momentum, energy and species mass fractions are solved by employing a one-step reaction mechanism and a $k-\omega$ turbulence model for the turbulent shear, heat-flux and diffusion terms. The numerical solutions are used to study the ignition process and the flame structure in an accelerating turbulent transonic mixing layer. Within the considered downstream distance growth rates of the turbulent accelerating reacting mixing layer are 5 to 20 times larger than in the corresponding laminar case. However, the characteristics of the flowfield are not changed by the turbulence. After ignition, a diffusion flame is established downstream from the splitter plate dividing the hot air stream and the fuel stream. The flame is slightly curved and angled towards the hot air stream. Variations in stream velocities, air temperature and pressure gradient in the downstream direction produce considerable variations in axial flame stand-off distance and ignition length. Local maxima in the oxygen concentration on the fuel side of the mixing layer and downstream from the splitter plate are found to result predominantly from the convection of significant amounts of oxygen, the latter being swept onto the fuel side in front of the flame. Free stream values of the specific dissipation rate are found to significantly change the growth rates of the mixing layer, but do not change the qualitative characteristics of the accelerating reacting flow.

Nomenclature

\begin{align*}
c_p & \quad \text{specific heat} \\
D & \quad \text{diffusivity} \\
h & \quad \text{enthalpy} \\
H & \quad \text{stagnation enthalpy} \\
h_t & \quad \text{total enthalpy} \\
h^o & \quad \text{heat of formation} \\
k & \quad \text{turbulent kinetic energy} \\
M & \quad \text{Mach number} \\
m & \quad \text{reaction rate} \\
N & \quad \text{total number of species} \\
Pr & \quad \text{Prandtl number} \\
p & \quad \text{pressure} \\
R & \quad \text{gas constant} \\
Sc & \quad \text{Schmidt number} \\
T & \quad \text{temperature} \\
u_{\infty} & \quad \text{free stream velocity at } y = \infty \\
u_{-\infty} & \quad \text{free stream velocity at } y = -\infty \\
u & \quad \text{velocity in } x\text{-direction} \\
v & \quad \text{velocity in } y\text{-direction} \\
x, y & \quad \text{Cartesian coordinates} \\
Y & \quad \text{mass fraction} \\
\rho & \quad \text{density} \\
\lambda & \quad \text{thermal conductivity} \\
\mu & \quad \text{coefficient of viscosity} \\
\nu & \quad \text{stoichiometric coefficient} \\
\rho & \quad \text{density} \\
\omega & \quad \text{turbulent dissipation rate} \\
\gamma & \quad \text{gamma} \\
\phi & \quad \text{phi} \\
\alpha & \quad \text{alpha} \\
\beta & \quad \text{beta} \\
c & \quad \text{c} \\
\delta & \quad \text{delta} \\
\theta & \quad \text{theta} \\
\varphi & \quad \text{varphi} \\
\in & \quad \text{in} \\
\approx & \quad \text{approximate} \\
\equiv & \quad \text{equivalent} \\
\frac{\partial}{\partial} & \quad \text{partial derivative} \\
\n & \quad \text{zero} \\
1 & \quad \text{one} \\
2 & \quad \text{two} \\
3 & \quad \text{three} \\
4 & \quad \text{four} \\
5 & \quad \text{five} \\
6 & \quad \text{six} \\
7 & \quad \text{seven} \\
8 & \quad \text{eight} \\
9 & \quad \text{nine} \\
a & \quad \text{a} \\
b & \quad \text{b} \\
c & \quad \text{c} \\
d & \quad \text{d} \\
e & \quad \text{e} \\
f & \quad \text{f} \\
g & \quad \text{g} \\
h & \quad \text{h} \\
i & \quad \text{i} \\
j & \quad \text{j} \\
k & \quad \text{k} \\
l & \quad \text{l} \\
m & \quad \text{m} \\
n & \quad \text{n} \\
o & \quad \text{o} \\
p & \quad \text{p} \\
q & \quad \text{q} \\
r & \quad \text{r} \\
s & \quad \text{s} \\
t & \quad \text{t} \\
u & \quad \text{u} \\
v & \quad \text{v} \\
w & \quad \text{w} \\
x & \quad \text{x} \\
y & \quad \text{y} \\
z & \quad \text{z}
\end{align*}

Subscripts

\begin{align*}
i & \quad \text{species (CH}_4, \text{O}_2, \text{N}_2, \text{CO}_2, \text{H}_2\text{O)} \\
\infty & \quad \text{quantity at the top far away from the layer} \\
-\infty & \quad \text{quantity at the bottom far away from the layer} \\
ref & \quad \text{quantity at reference condition} \\
t & \quad \text{turbulent quantity} \\
\end{align*}

Superscripts

\begin{align*}
\bar{} & \quad \text{(overbar) time-averaged or Reynolds-averaged value} \\
\tilde{} & \quad \text{(tilde) Favre-averaged value} \\
\end{align*}
Introduction

Accelerating reacting flows have recently become of interest in context with new compact designs of gas turbine engines or their combustors where the combustion process is extended beyond the combustion chamber into the flow through the turbine blades. Compact combustor design in combination with augmented burning in the turbine passage, has been shown, by thermodynamic analysis (Sirignano and Liu\(^1\)) to allow for (1) a reduction in after-burner length and weight, (2) a reduction in specific fuel consumption, and (3) an increase in specific thrust. Mixing and exothermic chemical reaction in an accelerating flow, such as the prescribed flow through a turbine passage, also promises benefits with respect to other combustion applications by reducing pollutant formation and heat transfer losses through the reduction of peak temperatures due to flow acceleration.

For zero pressure gradients, reacting multi-dimensional (laminar and turbulent) low Mach number mixing- and boundary-layer flows have been considered by many investigators using a wide variety of approaches. See, for example, Marble and Adamson\(^2\), Emmons\(^3\), Chung\(^4\) and Sharma and Sirignano\(^5\) for laminar flows, and Patankar and Spalding\(^6\) Razdan and Kuo\(^7\) and Givi et al.\(^8\) for turbulent flows.

Reacting supersonic flows have been considered by Buckmaster et al.\(^9\), Grosch and Jackson\(^10\), Jackson and Hussaini\(^11\), Im et al.\(^12,13\), and Chakraborty et al.\(^14\). For a two-dimensional, laminar, non-reacting, boundary layer over a solid body with a pressure gradient, similarity solutions were obtained by Li and Nagamatsu\(^15\), Cohen\(^16\) and Cohen and Reshotko\(^17\) who solved the momentum and energy equations transformed by the Illingworth-Stewartson transformation (Illingworth\(^18\), Stewartson\(^19\), Schlichting\(^20\)).

Sirignano and Kim\(^21\) reduced their partial differential equations to a system of ordinary differential equations, and obtained similarity solutions for laminar, two-dimensional, mixing, reacting and non-reacting layers with a pressure gradient that accelerates the flow in the direction of the primary stream.

Numerical solutions for the two-dimensional reacting mixing-layer equations without the use of the similarity assumptions were recently presented by Fang, Liu and Sirignano\(^22\) who compared their computational results with the similarity solutions obtained by Sirignano and Kim\(^21\) and extended their finite difference computations to non-similar cases, examining the ignition and combustion processes in a general transonic accelerating mixing layer.

The proposed analysis extends the work of Fang, Liu and Sirignano\(^22\) by including turbulence effects into the boundary-layer equations used by these authors.

Governing Equations

The two-dimensional steady case of a compressible viscous turbulent reacting mixing layer is considered in the presence of a pressure gradient. At the trailing edge of a flat splitter plate, hot air mixed with burned gases and flowing above the flat plate at velocity \(u_\infty\) comes into contact with fuel vapor flowing below the flat plate at velocity \(u_{\infty}\). The free streams can contain turbulent fluctuations in addition to the turbulence generated in the mixing layer. Upon contact of the two streams, chemical reactions take place between the air and the fuel vapor, and a diffusion flame will be established near the middle of the shear layer. The amount of burned gases in the initial mixture are considered parameters in the analysis, which can be varied from zero to a number determined by the temperature limitation on the flow.

We are concerned with the ignition and combustion that is established downstream of the point of initial contact between the accelerating fuel and air streams.

The boundary-layer approximation applied to the Favre averaged, compressible Navier-Stokes equations for a reacting flow then provides the following governing equations for axial momentum, energy and species mass fractions in the prescribed free shear or mixing layer

\[
\frac{\partial \tilde{u}}{\partial x} = -\tilde{v} \frac{\partial \tilde{u}}{\partial y} - \frac{1}{\rho_0} \frac{\partial p}{\partial x} + \frac{1}{\rho_0} \frac{\partial}{\partial y} \left[ \left( \mu + \mu_t \right) \frac{\partial \tilde{u}}{\partial y} \right] \tag{1}
\]

\[
\frac{\partial \tilde{Z}_j}{\partial x} = -\tilde{v} \frac{\partial \tilde{Z}_j}{\partial y} + \frac{1}{\rho_0} \frac{\partial}{\partial y} \left[ \left( \mu + \mu_t \right) \frac{\partial \tilde{Z}_j}{\partial y} \right], \quad j = 1, 2 \tag{2}
\]

\[
\frac{\partial Y_F}{\partial x} = -\tilde{v} \frac{\partial Y_F}{\partial y} + \frac{1}{\rho_0} \frac{\partial}{\partial y} \left[ \left( \mu + \mu_t \right) \frac{\partial Y_F}{\partial y} \right] + \frac{1}{\rho_0} \tilde{m}_F \tag{3}
\]

\[
\frac{\partial H}{\partial x} = -\tilde{v} \frac{\partial H}{\partial y} + \frac{1}{\rho_0} \frac{\partial}{\partial y} \left[ \left( \mu + \mu_t \right) \frac{\partial H}{\partial y} \right] + \frac{1}{\rho_0} \left( \mu + \mu_t \right) \frac{\partial}{\partial y} \left[ \frac{\partial (\tilde{u}^2/2)}{\partial y} \right] \tag{4}
\]

\[
\text{with the stagnation enthalpy}
H = \tilde{h}_t + \frac{1}{2} \tilde{u}^2 + k \tag{5}
\]
where $k$ is the turbulent kinetic energy and
\[
\tilde{h}_i = \int_{T_{ref}}^{T} c_p \, dT + \sum_{i=1}^{N} \tilde{Y}_i h_i^o
\]
(6)
or
\[
\tilde{h}_{i,t} = \int_{T_{ref}}^{T} c_{p,i} \, dT + \tilde{Y}_i h_i^o
\]
(7)
are the average total enthalpy or the total enthalpy of species $i$, with $c_{p,i}$ and $h_i^o$ being the specific heat and the heat of formation of species $i$ at the reference temperature $T_{ref}$. Here, each species $i$, i.e., $O_2$, $N_2$, $H_2O$, $CO_2$, and $CH_4$, was assumed to behave like an ideal gas. In Eq. (4) correlations involving fluctuations of $h_{i,t}$ have been neglected. $Y_F$ in Eq. 3 denotes the fuel mass fraction and $\bar{\nu}_F$ is the fuel consumption rate per unit mass. The latter has been eliminated by introducing the Shvab-Zeldovich variables:
\[
Z_j = Y_j - \nu_j Y_F, \quad j = 1, 2
\]
(8)
where $j = 1$ denotes air and $j = 2$ denotes products. Methane (CH$_4$) is used within the present work. The combustion process is described by a one-step overall chemical reaction, i.e.
\[
CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2
\]
(9)
with the reaction rate $k$ (in $cm^3$ mol sec kcal units) given by
\[
k = AT^n \, e^{-E_o/RT} [\text{Fuel}]^a [O_2]^b
\]
(10)
where $n = 0$ has been chosen in the present case. According to Westbrook and Dryer$^{23}$ for methane (CH$_4$), $A = 1.3 \cdot 10^9$, $E_o = 48.4 \, kcal/mol$, $a = -0.3$, $b = 1.3$. The effect of turbulence on the reaction rate has been neglected in this analysis. In particular, the turbulent reaction rate is computed from Eq. (10) by using the turbulent values of fuel and oxygen mass fraction or molar concentration. Note that, the turbulent length scale $l = \sqrt{\kappa/\omega}$ for case 0 in Table 1 is approximately 0.01 mm in the ignition region and 0.025 mm where the maximum temperature gradients occur. On the other hand, the ignition length in this case has been computed as 1.5 mm and the length across which the largest temperature gradient occurs is 0.8 mm. Therefore, the representation of the average reaction rate by the Arrhenius rate is reasonable.

The Prandtl number and the Schmidt number employed in Eqs. (4) and (3) are defined as
\[
Pr = \frac{c_p \mu}{\alpha}, \quad Sc = \frac{\mu}{\rho D}
\]

The Reynolds stress, turbulent heat-flux and turbulent transport of species $i$ have been modeled by employing the eddy viscosity $\mu$ and the turbulent Prandtl and Schmidt numbers, i.e., $Pr_i$ and $Sc_i$. Also, the diffusivity of all species $i$ was assumed to have the same value $D$. In Eqs. (1) through (7) an overbar (‘$\bar{}$’) denotes a time-averaged value and a tilde (‘$\tilde{}$’) indicates a Favre-averaged value.

The proposed implementation assumes $Pr_t = Sc_t = 0.5$ (even though different values might also be studied), and employs a standard $k - \omega$ turbulence model to evaluate the eddy-viscosity $\mu$, i.e.,
\[
\mu = \overline{\nu} k/\omega
\]
(11)

Accordingly, the additional equation for the turbulent kinetic energy $k$ and the specific dissipation rate $\omega$ are:
\[
\frac{\partial k}{\partial x} = -\frac{\partial}{\partial y} \left[ \frac{1}{\rho \overline{u} \overline{v}} \left( \frac{\partial \overline{u}}{\partial y} \right)^2 - \frac{1}{\overline{u}} \beta^t k\omega \right] - \frac{1}{\overline{u} \overline{v}} \left[ (\mu + \sigma^t \mu_t) \frac{\partial k}{\partial y} \right]
\]
(12)
\[
\frac{\omega}{\partial x} = -\frac{\partial}{\partial y} \left( \frac{1}{\rho \overline{u} \overline{v}} \left[ \frac{\omega}{k} h_t \left( \frac{\partial \overline{u}}{\partial y} \right)^2 - \overline{p}\omega^2 \right] \right) + \frac{1}{\rho \overline{u}} \left[ (\mu + \sigma_t \mu_t) \frac{\partial \omega}{\partial y} \right]
\]
(13)
whereby
\[
\alpha = 5/9, \quad \sigma = 1/2, \quad \sigma^t = 1/2
\]
(14)

Here, pressure work due to velocity fluctuations as well as pressure diffusion and pressure dilatation resulting from correlations of pressure fluctuations with velocity fluctuations or their gradients$^{24}$ have not been modeled.

Compressibility effects within the equations for $k$ and $\omega$ have been considered by varying the closure coefficients $\beta$ and $\beta^t$ with the turbulence Mach number $M_t = 2k/a^2$, where $a$ is the speed of sound$^{24}$
\[
\beta^t = \beta^t_o [1 + \xi^* F(M_t)]
\]
(15)
\[
\beta = \beta_o [1 + \xi F(M_t)]
\]
(16)
where $\beta^t_o = 9/100$ and $\beta_o = 3/40$ correspond to the values of $\beta^t$ and $\beta$ in the incompressible case. The values of $\xi^*$ and the compressibility function $F(M_t)$ have been chosen according to Ref. 24, i.e.,
\[
\xi^* = 1.5, \quad M_{t,o} = 0.25
\]
(17)
\[
F(M_t) = \left[ \frac{M_t^2 - M_{t,o}^2}{M_{t,o}^2} \right] H(M_t - M_{t,o})
\]
where \( \mathcal{H}(x) \) is the Heaviside step function.

For the perfect gas mixture resulting from the prescribed one-step reaction mechanism for methane-air diffusion flames, we get

\[
\dot{p} = \sum_{i=1}^{N} \rho_i R_i \dot{T} \tag{18}
\]

with the average gas constant \( R \) given by

\[
R = \sum_{i=1}^{N} R_i \dot{Y}_i \tag{19}
\]

Similarly, the average specific heat and the average viscosity coefficient are calculated from the specific heat and viscosity coefficient of each species \( c_{p,i} \) and \( \mu_i \), i.e.,

\[
c_p = \sum_{i=1}^{N} c_{p,i}(\dot{T}) \dot{Y}_i \tag{20}
\]

\[
\mu = \sum_{i=1}^{N} \mu_i(\dot{T}) \dot{Y}_i \tag{21}
\]

whereby the temperature dependence of the \( \mu_i \)’s is approximated by using Sutherland’s formula. The specific heats \( c_{p,i} \) are obtained from polynomial approximations to tabulated values of \( c_{p,i} \) as a function of temperature.

**Solution Method and Constraints**

The solution algorithm for the prescribed steady, two-dimensional, turbulent reacting mixing layer is based on the solution method proposed by Fang, Liu and Sirignano but extended for turbulent flows and augmented by the governing equations for \( k \) and \( \omega \). Fang et al. proposed a parabolic Crank-Nicholson type marching scheme to study a laminar reacting mixing layer using a one-step reaction mechanism. Their method is second-order accurate in both the \( x \)-direction and the \( y \)-direction. Each integration step in the axial direction involves the simultaneous solution of the governing equations at each transverse grid point and the use of appropriate free stream conditions in the transverse flow direction, i.e. \( \tilde{u} \rightarrow u_{\pm \infty} \), \( H \rightarrow H_{\pm \infty} \), \( Z_j \rightarrow Z_j_{\pm \infty} \), \( Y_F \rightarrow Y_{F,\pm \infty} \), \( k \rightarrow k_{\pm \infty} \) and \( \omega \rightarrow \omega_{\pm \infty} \) as \( y \rightarrow \pm \infty \).

To march out the solution in the \( x \)-direction, inflow conditions on both sides of the splitter plate have to be specified, as well as boundary conditions in the transverse direction away from the mixing layer. The latter involves the specification of free stream conditions for both oxidizer stream and fuel stream.

At each integration step \( i \) in the \( x \)-direction, we first solve for the velocity in the \( x \)-direction \( \tilde{u} \), temperature \( \tilde{T} \) (as described below), turbulent quantities \( k \) and \( \omega \) and the mass fractions for all seventeen species. This step involves the simultaneous solution of the governing equations at each transverse computational node by using flow parameters evaluated at the previous integration step, i.e., at \( i-1 \). Then, we calculate the density \( \rho \) and the velocity in the transverse direction \( \tilde{v} \) at the \( i \)th step by employing the equation of state and the continuity equation using the new solutions. After the solutions for all dependent variables at \( i \) have been obtained, we re-iterate the solution by solving the partial differential equations again using the mean values of parameters at the current step \( i \) and the previous step \( i-1 \). Re-iteration continues until the differences between the solutions of the current and the previous iteration are below a certain cut-off for the fuel mass fraction or the temperature.

For the cases that are analyzed, both Prandtl and Schmidt numbers, i.e., \( Pr \) and \( Sc \), are assumed constant throughout the simulation. The pressure gradient leading to stream acceleration in the axial or \( x \)-direction is expressed in terms of the free-stream velocity, i.e.,

\[
-\frac{dp}{dx} = \rho_{\pm \infty} u_{\pm \infty} \frac{du_{\pm \infty}}{dx} \tag{22}
\]

where the subscript \( \pm \infty \) denotes values of the corresponding free stream, at large distances (in positive + or negative − \( y \)-direction) away from the mixing layer.

The velocity component in the \( y \)-direction \( \tilde{v} \) can be obtained by integrating the continuity equation (starting at \( y = -\infty \)), once \( \tilde{u} \) has been determined within the flowfield. This yields

\[
\rho_{\pm \infty} \tilde{v} = \int_{y=-\infty}^{y} \frac{\partial (\rho_{\pm \infty} \tilde{u})}{\partial x} dy'. \tag{23}
\]

Defining \( \tilde{h} \) as

\[
\tilde{h} = \sum_{i=1}^{N} \tilde{h}_i \dot{Y}_i = \int_{T_{ref}}^{T} \sum_{i=1}^{N} c_{p,i} \dot{Y}_i d\Gamma' \tag{24}
\]

with

\[
\tilde{h} = H - \frac{1}{2} \tilde{u}^2 - k - \sum_{i=1}^{N} \dot{Y}_i \tilde{h}_i^0 \tag{25}
\]

an incremental change of \( \tilde{h} \), i.e., \( d\tilde{h} \) is given by

\[
d\tilde{h} = \sum_{i=1}^{N} \frac{\tilde{Y}_i}{\dot{Y}_i} d\tilde{T}_i + c_m d\tilde{T} \tag{26}
\]

from which the temperature change \( d\tilde{T} \) is obtained. This allows the determination of the temperature \( \tilde{T} \) at each integration step \( \tilde{T} \) (at all discrete \( y \) locations) starting with the integration at the trailing edge of the splitter plate where the mixture of hot air and burned gases (flowing above the flat plate) at velocity \( u_{\infty} \) comes into contact with fuel vapor flowing below the flat plate at velocity \( u_{-\infty} \).
Results of the Numerical Investigation

Non-Reacting Turbulent Mixing Layer

The laminar version of the proposed numerical method has been benchmarked by Fang, Liu and Sirignano\textsuperscript{22} against the similarity solutions found by Sirignano and Kim\textsuperscript{21} for both non-reacting and reacting cases. In order to validate the implementation of the $k$-$\omega$ turbulence model, computed results for the non-reacting single component mixing layer have been compared with those predicted numerically by Wilcox\textsuperscript{24} and observed experimentally by Liepmann and Laufer.\textsuperscript{27} (See Ref. 24, Figure 3.4.) The flowfield behind a splitter plate dividing quiescent ambient air from an airstream at low Mach number is considered. See Ref. 24, Figure 3.4. The comparison illustrated in Fig. 1 shows that the present implementation predicts the spreading rate of the mixing layer very well on the side of the airstream. On the opposite side, the spreading rate is overpredicted by about 10\% of the total spreading rate. The nondimensional velocities in the center of the mixing layer are predicted too low (with a maximum error of 10 per cent). Note that in the present simulation $y = 0$ denotes the location of the splitter plate, and the location where $U/U_{\text{max}} = 0.5$ is located at $y/x = -0.014$. Free stream values for $k$ and $\omega$ have been chosen according to the suggestion by Wilcox for the mixing layer configuration, i.e. $k = 2.5 \times 10^{-5} \text{m}^2/\text{s}^3$ and $\omega = 500 \text{s}^{-1}$.

Turbulent and Laminar Reacting Mixing Layer

In order to illustrate the relevance of turbulent transport, the ‘base case’ condition previously analyzed by Fang, Liu and Sirignano\textsuperscript{22} has been considered. In this case a hot air stream (situated above the flat plate at $y > 0$ mm) at velocity $u_{\infty} = 50$ m/s and temperature $t = 1650$K comes into contact with a fuel vapor stream below the plate at velocity $u_{-\infty} = 25$ m/s and temperature $t = 400$ K. A schematic diagram of the configuration is shown in Fig. 2. Both streams are accelerated due to a pressure gradient of $dp/dx = -200 \text{N/m}^2$. The static pressure in both streams at $x = 0$ mm is $p = 30$ atm. Figs. 3 and 4 illustrate velocity and temperature profiles for the turbulent and non-turbulent cases at various downstream positions. For the case where turbulent transport has been considered, the same free stream values for $k$ and $\omega$ have been imposed as for the prescribed non-reacting mixing layer. In the turbulent case the spreading of momentum at $x = 12.5$ mm is on the air side ($y > 0$ mm) 5.4 times larger and on the fuel side ($y < 0$ mm) 11 times larger than in the laminar case. At $x = 37.5$ mm the multiplication factors have increased to 15 on the air side and 23 on the fuel side, respectively. Similarly, the growth of the thermal boundary layer is significantly larger than in the laminar case. At $x = 12.5$ mm, the spreading of the temperature profile on the air side is 5.8 times larger and on the fuel side 12.5 times larger than in the laminar case. At $x = 37.5$ mm, the factors have increased to 14.4 on the air side and 22.9 on the fuel side. Here, spreading of velocity or temperature profiles in the $y$-direction is measured from $y = 0$ mm up to the $y$-location where these variables take their undisturbed free stream values.

Fig. 5 shows the density profiles for both turbulent and non-turbulent cases at different axial locations. Figs. 3 and 5 show that the boundary layer grows in the downstream direction and the ratio $u_{\infty}/u_{\text{mix}}$ becomes slightly larger. The species mass fractions of $O_2$, $N_2$, $CO_2$, $H_2O$, and $CH_4$ for the turbulent case, subsequently referred to as base case or case 0, are shown in Fig. 6. Even though the spreading of the turbulent boundary layer is significantly larger than that found in the laminar case, the characteristics of the reacting methane-air mixing layer, are not changed by the presence of turbulent diffusion. Fig. 7 shows temperature contours computed for the prescribed base case. One observes that ignition occurs after a certain distance downstream from the end of the splitter plate after the hot air and the fuel vapor have met. Figure 8 is a close-up view of the temperature contours near the ignition region. Temperature profiles versus $y$ for the base case at four different $x$ positions were already illustrated in Fig. 4. The peak temperature occurs at a positive value of $y$ (the air side) and is moving upward as the flow moves downstream. This observation can be explained by the fact that, in stoichiometric combustion, the mass of air required is much greater than that the mass of fuel. The density profiles $\bar{\rho}(y)$ for the base case shown in Fig. 5 have a minimum where the temperature is high. Note however that in this analysis, the pressure at the same $x$-location is constant in the $y$-direction.

Density and velocity on the air side remain larger than on the fuel (CH\textsubscript{4}) side. Absolute values for the velocity $\bar{u}$ at $x = 12.5$ mm, 25 mm, 37.5 mm and 50 mm are illustrated in Fig. 9. In Fig. 5, the density minima near the middle of the shear layer (i.e. where the reaction takes place) results, due to the same pressure gradient across the mixing layer, in an increased flow acceleration compared to the acceleration of the two free streams. Therefore, the nondimensional velocity curves illustrated in Fig. 3 peak at the same $y$-position as the maximum temperature and minimum density in Figs. 4 and 5. The maximum in the profile for product mass fraction illustrated in Fig. 6 also occurs at the same $y$-location as those for the prescribed flow quantities. There is a local maximum in the $O_2$ mass fraction slightly below $y = 0$ mm. Fang, Liu and Sirignano\textsuperscript{22} explained this by noting that at some $y$ position the density increase in $O_2$ due to diffusion is greater than the mass fraction of $O_2$ consumed by the chemical reaction. However, as can be observed from the contour lines for the $O_2$ mass fraction in Fig. 10,
the O₂ mass fraction on the fuel side of the flame, seems to result predominantly from the convection of significant amounts of O₂, the latter being swept onto the fuel side in front of the flame. Note that at \( x = 0 \) mm, the mixing layer is located at \( y = 0 \) mm whereas the flame establishes itself at \( x = 7 \) mm downstream and \( y = 0.18 \) mm above the edge of the splitter plate.

Contour plots of the turbulent kinetic energy \( k \) and the specific dissipation rate \( \omega \) are shown in Figs. 11 and 12. Maximum values for \( k \) at \( x = 12.5 \) mm and \( x = 50 \) mm are \( k = 730 \text{m}^2/\text{s}^2 \) and \( k = 379 \text{m}^2/\text{s}^2 \), respectively. At the same \( x \)-positions \( \omega \)-values are \( 3.11 \cdot 10^5 \text{s}^{-1} \) and \( 6.16 \cdot 10^5 \text{s}^{-1} \), respectively. Also, within \( x = 12.5 \) mm and \( x = 50 \) mm, maxima of \( k \) slightly shift towards the fuel side \((y < 0 \text{ mm})\) in the downstream direction. However, in the same range of \( x \)-positions, maximum values of \( \omega \) slightly shift from the fuel side at \( x = 12.5 \) mm onto the centerline \((y = 0 \text{ mm})\) at \( x = 50 \) mm. Figure 13 shows Mach number profiles versus \( y \) at four different \( x \)-positions. The Mach number profiles for a given \( x \)-location reach a minimum where the temperature peaks, i.e. where the speed of sound is high. This behavior is also evident in Ref. 22. A second local minimum in the Mach number profiles as observed by Fang, Liu and Sirignano in the laminar case is not found in the turbulent simulation. Note that in the considered domain \( x = 0 - 50 \) mm, the flow remains subsonic. A Mach number of one is first reached in the free stream at \( x = 70 \) mm (not illustrated). At this location the Mach number within the flame is still subsonic with a maximum of approximately 0.8. Contour lines for the mass fraction of products are shown in Fig. 15. It is clear that shortly after ignition local product concentration is determined by both reaction rate and diffusion. Further downstream, however, where the flame is established, local product concentration is determined predominantly by diffusion. This might partly explain the slight bending of the contour lines for the product mass fraction near the flame front at \( x = 7 \) mm.

**Parametric Studies / Turbulent Reacting Mixing Layer**

In this section we study the influence of various flow parameters on ignition and flame structure. Table 1 lists the different cases of the study including the base case (case 0) considered in the previous section. Cases 1 through 12 represent a set of cases for each of which one flow parameter, i.e. air temperature, pressure gradient, fuel velocity, air velocity, free stream turbulent kinetic energy or free stream specific dissipation rate, has been modified relative to the base case configuration (case 0) discussed in the previous section. For all cases \((0 - 12)\), the static inlet pressure at \( x = 0 \) mm is \( p_0 = 30 \text{ atm} \) and the fuel inlet temperature \( 400 \text{ K} \). The computational grid size for all cases was \( \Delta x = 0.03125 \text{ mm} \) and \( \Delta y = 0.015 \text{ mm} \), except for cases 4 and 7 with \( \Delta x = 0.00625 \text{ mm} \) and \( \Delta y = 0.0075 \text{ mm} \).

**Initial Air Temperature:**

In case 1, the initial air temperature is decreased from \( T_{air} = 1650 \text{ K} \) to \( T_{air} = 1350 \text{ K} \). Velocity and temperature profiles for this case at various \( x \)-locations are shown in Figs. 16 and 17. Mixing-layer growth in both transverse directions is smaller than in the base case. Since the temperature on the hot air side is too small to ignite the fuel-air mixture within the mixing layer, there is no acceleration of the flow due to ignition and consequently, no local maximum is observed within the velocity profiles in the transverse direction. Also, the point where all illustrated velocity profile curves cross each other now lies at \( y = 0 \) mm and no longer on the air side \((y < 0 \text{ mm})\) as observed in the base case.

Due to the lower air temperature, the air density in the free stream remains larger than in the base case (at the corresponding axial location), but acceleration of the air stream in the downstream direction is less than in the base case. Acceleration of the fuel stream is not significantly influenced by the decrease in air temperature. Analogous to the momentum layer, the growth of the thermal layer is significantly less than observed in the base case. The free stream density on the fuel side along the mixing layer remains virtually unchanged by the decrease of the inflow air temperature. Again, due to the lack of ignition the temperature and density profiles in the transverse direction are monotonic without local maxima or minima as found in the base case.

At corresponding \( x \)-positions, values of the turbulent kinetic energy \( k \) are about three times smaller than in the base case. This can also be observed from the contour plot of \( k \) shown in Fig. 18. Maxima in \( k \) are slightly shifted to the air side, whereas in the base case, maxima in \( k \) are slightly shifted to the fuel rich side \((y < 0 \text{ mm})\). Maximum values of \( \omega \) are about \( 2/3 \) of the corresponding values in the base case. Also, maximum values of \( \omega \) slightly shift towards the fuel rich side. At \( x = 12.5 \) mm the maximum is located at about \( y = 0.25 \text{ mm} \), at \( x = 50 \) mm the maximum is found at \( y \approx 0 \), i.e. the \( y \)-location of the splitter plate. Recall that, in the base case at \( x = 12.5 \) mm, the maxima in \( \omega \) is situated slightly on the fuel rich side and shifts towards \( y = 0 \) mm further downstream (approaching \( y = 0 \) mm at \( x = 50 \) mm).

The mass fractions of reaction products \((\text{CO}_2 \text{ and H}_2\text{O})\) remain zero due to the lack of ignition. According to the reduced growth of the mixing layer, diffusion of \( \text{CH}_4 \) on the fuel side and \( \text{N}_2 \) on the air side is reduced and the corresponding gradients in these regions remain larger than in the base case. However, due to the lack of ignition and a reaction zone, \( \text{CH}_4 \) and \( \text{O}_2 \) diffuse further into the opposite stream (i.e. fuel side for \( \text{O}_2 \) and air side for \( \text{CH}_4 \)) than in the base case. See Fig. 19.
In case 2, the initial air temperature is increased from $T_{\text{air}} = 1650\,\text{K}$ to $T_{\text{air}} = 1950\,\text{K}$. The growth rate of the mixing layer on the air side is about the same as in the base case, whereas its growth on the fuel side is slightly larger in comparison to the base case. Acceleration of the air stream increases with the increase in air stream temperature. The velocity of the free stream air at $x = 50\,\text{mm}$ is about 660 m/s, in contrast to 610 m/s for the base case. However, local maxima of the nondimensional velocity (i.e., velocity normalized by the velocity of the free stream $u_{+\infty}$) are smaller than in the base case at the same $x$-position.

Due to the increased air temperature, overall density values on the air side are smaller than in the base case. The same is true for the local density minimum found within the combustion zone of the mixing layer when plotting $T$ versus $y$. Even though, the growth of the mixing layer on the air side is about the same as in the base case, local minima for the density are shifted towards the air side (Fig. 20).

The similar observation made for the local minimum values of density, can be made within the temperature profiles (again in the transverse direction). Even though the growth of the thermal layer on the air side is about the same as in the base case (see Table 2), locations for the maximum temperatures are shifted towards the air side (see Fig. 21). This agrees with the observed increase of the maximum temperature value at a given $x$-position of about 90 per cent of the increase in the free stream temperature at that same downstream location. Note that, with the exception of case 2, the maximum flame temperature in all other cases is approximately the same, i.e., $T_{\text{max}} \approx 3050\,\text{K}$, whereas for case 2, $T_{\text{max}} \approx 3250\,\text{K}$. The decrease in the maximum temperature downstream from the location where $T_{\text{max}}$ is reached (i.e., slightly downstream from the location where the temperature gradient is a maximum) is approximately the same in all considered cases, i.e., 2.5 K/mm.

Values of the turbulent kinetic energy $k$ are slightly larger in the base case, ranging between 5% (at $x = 12.5\,\text{mm}$) and 20% (at $x = 50\,\text{mm}$). Maximum values shift slightly towards the air side in the downstream direction, whereas the shift is towards the fuel side in the base case (case 0). Values for $\omega$ are slightly larger at $x = 12.5\,\text{mm}$ than in the base case. Further downstream, maximum $\omega$ values drop slightly below the corresponding base case values due to increased spreading of both $\omega$ and $k$ on the fuel side. Maximum values of $\omega$ are found at $y = 0\,\text{mm}$, whereas in the base case, maximum values of $\omega$ shift slightly from the fuel side (e.g., at $x = 12.5\,\text{mm}$) towards $y = 0\,\text{mm}$. At $x = 50\,\text{mm}$, the flame center (e.g., location of maximum temperature or location of maximum product mass fraction) is shifted approximately 0.4 mm towards the air side, in comparison to the flame center location in the base case. Accordingly, gradients of $\text{CH}_4$ are smaller and gradients of $\text{O}_2$ are larger than in the base case. However, due to the prescribed increased growth of the mixing layer (on the fuel side), product concentrations and $\text{N}_2$ concentrations on the fuel side (below $y = -1\,\text{mm}$) are larger than in the base case. The mass fraction of $\text{O}_2$ at $x = 50\,\text{mm}$ is significantly reduced compared to its base case value.

### Pressure Gradient:

The imposed reduction of the pressure gradient from absolute value of 200 N/m² to an absolute value of 50 N/m³ leads in case 3 to a significant reduction in both air and fuel stream velocities, approximating 190 m/s on the fuel side and 200 m/s on the air side at $x = 50\,\text{mm}$. The corresponding base case values are 400 m/s and 610 m/s, respectively. The ratio of $u_{-\infty} / u_{+\infty}$ is smaller than in the base case.

The transverse location where all normalized velocity profiles have the same value is found at $y = 0\,\text{mm}$, whereas in the base case this location is less distinct and is found to be situated slightly on the side of the mixing layer. Despite the reduced free stream acceleration, maximum values of the normalized velocity (i.e., $\bar{u}_{\text{max}} / u_{+\infty}$) are smaller ($0\% - 25\%$ between $x = 12.5\,\text{mm}$ and $50\,\text{mm}$) than those predicted for the base case. However, maximum values occur approximately at the same $y$-positions as in the base case. On the air side, growth of the mixing layer is smaller than in the base case; on the fuel side, it is larger at $x = 12.5\,\text{mm}$, but smaller at $x = 25, 37.5$ and $50\,\text{mm}$.

Due to the reduced flow acceleration, free stream values of both air and fuel density remain larger than in the base case. Spreading of the density profiles follows the prescribed growth of the mixing layer. Also, density minima are found approximately at the same $y$-location as in the base case at the corresponding $x$-position. However, in contrast to the base case, minimum density values decrease only very little in the downstream direction (within $x = 12.5 - 50\,\text{mm}$). The decrease of the free stream temperatures due to stream acceleration is much smaller than in the base case, this holds particularly true for the fuel stream. The transverse temperature profiles are very similar to those for the base case at the same $x$-position, with the exception of the local minimum temperature values which analogous to the density minima remain almost constant for the various $x$-locations. See Figs. 22 and 23. The predicted values for $k$ are only $25\% - 33\%$ of those found in the base case at the same $x$-position. Spreading of $k$ in the fuel region is the same as in the base case but less in the air region (Fig. 24). $\omega$ values are about one-half of those for the base case. Analogous to the base case, maxima values of $\omega$ shift from the fuel side (at $x = 12.5\,\text{mm}$) onto the $y = 0\,\text{mm}$ position at $x = 50\,\text{mm}$. At $x = 50\,\text{mm}$, the location...
where CH₄ and O₂ are totally consumed and where the product concentration has a maximum value is approximately the same as in the base case. Note that in Table 1, the flame angle for case 3 is the same as the base case (case 0). Profiles for O₂ and CH₄ at x = 50 mm differ only slightly in comparison to the base case. However, there is less diffusion of products into the air side, i.e., at y-values beyond that of maximum product concentration. In the same region the gradients of oxygen mass fraction are larger. Also, in contrast to the base case, there is no significant amount of O₂ found on the fuel side at x = 50 mm.

In case 4, the absolute value for the pressure gradient was increased from 200 N/m³ to 330 N/m³. Air and fuel stream acceleration is increased, yielding free stream velocities of 500 m/s on the air side and 330 m/s on the fuel side at x = 20 mm. In the base case free stream velocities of air and fuel at x = 25 mm are 410 m/s and 275 m/s, respectively.

Profile plots of the nondimensional axial velocity versus transverse direction for various x-locations, do not show a common y location where all profiles cross. Recall that, the latter has been found in the base case and even more so for case 3. Predicted maximum values of the nondimensionalized velocity (\(\tilde{u}_{\text{max}}/u_{\infty}\)) between x = 12.5 mm and x = 50 mm are larger than in the base case, i.e., about 50 % of (\(u_{\text{max}}/u_{\infty} - 1\)). Predicted growth of the mixing layer is larger than in the base case (on both air and fuel side). However, the spreading rate of product mass fraction shown in Table 2 is slightly smaller than in the base case. Locations where the axial velocity profiles versus y reach their maximum are slightly shifted towards the air side from their base case positions. The ratio of the two free stream velocities does not significantly vary from its base case value.

The increased free stream acceleration yields smaller density values in both air and fuel streams in comparison to the base case. This is particularly true at larger downstream locations, e.g., \(x = 37.5\;\text{mm}\) and 50 mm. Minimas of density profiles along \(x = \text{const}\). lines are shifted towards the air side. However, the decrease of the local density minima at a given x-position in comparison to its base case value is found to be less than the decrease of the free stream air density compared to its corresponding base case value. For the considered fuel, the decrease of free stream density downstream from the splitter plate in comparison to the base case is larger on the fuel side than on the air side of the mixing layer.

In contrast to the base case, and analogous to the previous discussion of the axial velocity profiles, no common y position is found where the temperature value is the same at different x-positions. Due to the increased free stream acceleration, free stream temperatures on both sides of the mixing layer are slightly lower than in the base case, particularly at \(x > 12.5\;\text{mm}\). Growth of the thermal layer on both air side and fuel side is larger than in the base case. This also holds true for the spreading rate of the product mass fraction shown in Table 2. According to the increased flame angle (see Table 1) locations of maxima in transverse temperature profiles are found at larger y-positions than in the base case. Maximum temperatures at a given x-location are only slightly smaller (i.e., 50 - 200 K within \(x = 12.5 - 30\;\text{mm}\)) than in the base case. Temperature contours in the ignition region are shown in Fig. 25.

For the considered x-locations (i.e., \(x = 12.5\;\text{mm}, 25\;\text{mm}, 37.5\;\text{mm}, 50\;\text{mm}\)), maximum \(k\)-values are approximately two times larger than the corresponding base case values with a 30 % increase in the spreading rate of \(k\) on both air and fuel sides. As for the base case, \(k\)-profiles are not symmetric along the y = const. line on which the splitter plate is located. This is particularly true close to the location of the flame front (Fig. 26). Maximum \(\omega\)-values at the prescribed locations are predicted to exceed their base case values by 20 % - 30 %. At \(x = 20\;\text{mm}\) the location of the flame center is shifted about 0.1 mm towards the air side (compared to the base case). As shown in Fig. 27, a significant amount of oxygen is swept on the fuel side, i.e., below the flame, before the flame is established. Consequently a significant oxygen mass fraction is found at \(x = 20\;\text{mm}\) as shown in Fig. 28. Subsequently, this oxygen will be partly consumed by the flame but also diffused as it is propagated downstream. The resulting maximum oxygen mass fraction at \(x = 50\;\text{mm}\) is well below the value predicted for the base case.

**Air Velocity:**

In case 5, the velocity of the air stream has been decreased from \(u_{\text{air}} = 50\;\text{m/s}\) to \(u_{\text{air}} = 30\;\text{m/s}\). The free stream fuel velocities at \(x = 12.5\;\text{mm}\) and higher remain virtually unchanged by this reduction of the initial free stream air velocity. However, whereas the ratio \(u_{-\infty}/u_{+\infty}\) slightly increases in the base case, it now remains virtually constant. Growth of the mixing layer is predicted to be larger than in the base case: Spreading of the velocity defect at \(x = 37.5\;\text{mm}\) on the air side, is 25 % larger than in the base case, and 19 % larger on the fuel side. Maximum temperatures at the considered downstream positions (\(x = 12.5, 25, 37.5, 50\;\text{mm}\)) are approximately the same as in the base case but shifted towards the air side (e.g., approx. 0.2 mm at \(x = 50\;\text{mm}\)) in accordance with the larger flame angle (see Table 1). Maximum \(k\)-values are somewhat larger than in the base case (approx. 317 m²/s² at \(x = 37.5\;\text{mm}\)). Maximum \(\omega\)-values are predicted to be smaller at the same x-position (approximately \(7 \cdot 10^4\;\text{s}^{-1}\)). Contour plots of \(k\) and \(\omega\) are shown in Figs. 29 and 30. Note that \(\omega\) in this case has a local
maximum at \(x \approx 10\) mm, if plotted versus \(x\) at \(y = 0\) mm. Maximum product concentration at \(x = 20\) mm is observed about 0.1 mm further on the air side than in the base case. The spreading rate for the product mass fraction is larger than in the base case (see Table 2). Oxygen mass fraction at \(x = 50\) mm is negligible compared to the amount predicted in the base case.

For case 6 where \(u_{\text{air}}\) is increased from \(u_{\text{air}} = 50\) m/s to \(u_{\text{air}} = 100\) m/s, the nondimensional velocity ratio \(u_{\text{max}}/u_{\infty}\) at \(x = 12.5, 25\) mm and 37.5 mm is slightly below the base case value, however, at \(x = 50\) mm the same value is reached as in the base case. Spreading of the velocity defect on the air side is found to be the same as in the base case, but slightly larger on the fuel side. Velocity contour lines for this case are illustrated in Fig. 31. At \(x = 12.5\) mm the peak within the density profile \(\rho(y)\) is found to be narrower, and the minimum value slightly smaller than in the base case. However, further downstream density profiles \(\rho(y)\) vary only slightly from the base case profiles. Temperature profiles \(T(y, x = \text{const})\) do not exhibit significant differences in comparison to the base case profiles. Maximum \(k\) values are slightly larger (0(10^5)) and maximum \(\omega\) values slightly smaller (0(10^4)) than in the base case. The flame angle 1.44° is smaller than the base case value 1.5°. The maximum O2 mass fraction on the fuel side at \(x = 50\) mm is larger than in the base case (see Fig. 32).

**Fuel Velocity:**
A reduction in the free stream fuel velocity (\(u_{\infty}\)) in case 7 yields an increase in the maximum value of the nondimensional velocity profile \(\bar{u}(y)/u_{\infty}\) in comparison to the value predicted for the base case at the same \(x\)-location. Growth of the mixing layer is faster than for the base case. While local density minima for \(\rho(y, x = \text{const})\) within \(x = 12.5 - 50\) mm are about the same as in the base case, they are slightly shifted towards the air side (\(\Delta y = 0.12\) mm at \(x = 50\) mm). The growth of the thermal layer is also increased with a shift of the maximum temperature values towards the air side. Maximum values of temperature profiles versus \(y\) are slightly larger (\(\approx 60\) K) than for the base case at corresponding \(x\)-locations. Note that the flame angle shown in Table 1 with 1.39° is smaller than the base case value. However, this angle is the approximate flame angle at \(x = 20\) mm. (Note the asterisk ‘*’ in Table 1.) In fact, in all the considered cases, the flame is slightly curved towards the air side; its angle at an \(x\)-position slightly larger than the flame stand-off distance \(x_H\) is somewhat smaller than the approximate flame angle further downstream (e.g. at \(x = 40\) mm). Note that all flame angles in Table 1 are evaluated at \(x = 40\) mm, with exception of cases 4 and 7. The flame stand-off distance as observed from Fig. 33 is approximately \(x_H = 4.8\) mm, approximately 30% smaller than in the base case. \(k\)-values are slightly larger (e.g. by 250 m^2/s^2 at \(x = 37.5\) mm) and \(\omega\) values slightly smaller (e.g. by 5 \cdot 10^4 at \(x = 37.5\) mm) than their base case counterparts. Due to the increased mixing layer growth rate, gradients in CH4, N2 and those of the product species at \(x = 50\) mm are smaller than in the base case. The location of maximum product mass fraction is slightly shifted towards the air side in comparison to its location in the base case (i.e. by 0.2 mm at \(x = 50\) mm). In contrast to the base case, there is no significant amount of oxygen present on the fuel side at \(x = 50\) mm. Fig. 34 illustrates the species mass fractions at \(x = 20\) mm. Note that the local maximum in the oxygen mass fraction at \(y < 0\) mm is significantly smaller than that observed at the same location for case 4 (see Fig. 28). This is simply due to the shorter flame stand-off distance in this case, allowing less oxygen to traverse in front of the flame across the \(y = 0\) mm line. Interestingly, even though the flame stand-off distance in case 4 is larger than for the base case, the O2 mass fraction at \(x = 50\) mm is significantly lower than for the base case.

In case 8, the relative velocity between the air and fuel stream has been decreased by increasing the fuel velocity from \(u_{\text{fuel}} = 25\) m/s to \(u_{\text{fuel}} = 45\) m/s. Despite this increase in the initial fuel stream velocity, the absolute free stream velocity values at \(x = 12.5\) mm and larger show on little differences from the base case values. However, the ratio of \(u_{\infty}/u_{\infty}\) slightly decreases in the downstream direction, whereas it slightly increases in the base case. Maximum values of the nondimensional velocity \(u_{\infty}/u_{\infty}\) are somewhat larger than in the base case. The mixing layer grows faster than under base case conditions (see Figs. 35, 36). In comparison to the case with decreased free stream fuel velocity (case 7), mixing layer growth is the same on the air side, but less on the fuel side. The free stream temperatures on both sides for \(x > 12.5\) mm remain virtually unchanged by an increase in the free stream fuel velocity. The free stream fuel temperature decreases by about 30K from \(x = 12.5\) mm to 50 mm, but the temperature decrease on the air side is approximately 113 K. \(k\)-values are found to be slightly larger than in the base case but the increase is smaller than that found for case 7. Similarly, maximum values of \(\omega\) are predicted to be slightly smaller than for the base case, but larger than for the case with reduced fuel stream velocity (case 7). The location of the maximum mass fraction for products CO2 and H2O at \(x = 50\) mm is slightly shifted from its base case location towards the air side, but less than predicted for case 7. The mass fraction of oxygen in the fuel stream at \(x = 50\) mm is small compared to the amount predicted for the base case.

**Free Stream Turbulent Kinetic Energy:**
With a decrease in the free stream turbulent kinetic energy from \(k = 2.5 \cdot 10^{-4} \text{ m}^2/\text{s}^2\) to \(k = 2.5 \cdot 10^{-6} \text{ m}^2/\text{s}^2\)
in case 9, mixing layer growth is found to be smaller than in the base case. Spreading of the velocity defect at \( x = 37.5 \) mm is 19% smaller on the air side and 16% smaller on the fuel side in comparison to the base case. Close to the splitter plate, i.e. at \( x = 12.5 \) mm and 25 mm, predicted maximum values for the nondimensional axial velocity are 20% smaller than \( (u_{\text{max}} - u_{\infty})/u_{\infty} \) for the base case. Maxima for velocity profiles \( \bar{u}(y) \) within \( x = 12.5 - 50 \) mm are predicted to be about 0.15 mm closer to the \( y = 0 \) mm line than in the base case. Minima for density profiles \( \bar{\rho}(y) \) at a given \( x \)-location have approximately the same value as in the base case but as for the velocity maxima, the values are shifted by about 0.15 mm towards the fuel side.

The growth of the thermal mixing layer is reduced. The common \( y \)-location where all temperature profiles \( T(y) \) have the same value is preserved (see Fig. 37). However, and in contrast to the base case, the same is not true for the transverse velocity profiles \( \bar{u}(y) \). The maximum temperature at \( x = 27.5 \) mm is now larger than that at 12.5 mm. The inverse was true in the base case. According to the reported shift in the maximum values of \( \bar{\rho} \) and \( \bar{u} \), the maximum temperature locations and maximum product concentration locations are both shifted towards the fuel side by about 0.15 mm within \( x = 12.5 \) mm and \( x = 50 \) mm. This agrees with the observed flame angle of 1.35° (see Table 1) which is smaller than the base case value. Maximum \( k \) values are found to be 7% (at \( x = 50 \) mm) - 15% (at \( x = 12.5 \) mm) smaller than in the base case. Within the same range of \( x \)-values, maximum \( \omega \)-values are 16% - 50% larger than the base case values. The maximum value for the mass fraction of products at \( x = 50 \) mm is approximately the same as in the base case, i.e. 0.26. In fact, approximately the same value is found in all the cases 0 - 12.

Due to the reduced mixing-layer growth overall gradients for the mass fractions of \( O_2 \), \( CH_4 \), products, and \( N_2 \) near the flame are larger than in the base case. Mass fractions of \( N_2 \) and product mass fractions on the fuel side are smaller, and \( CH_4 \) mass fractions are larger than their base case values. At \( x = 50 \) mm, no significant amount of oxygen is found on the fuel side.

An increase of the free stream turbulent kinetic energy in case 10 from \( k = 2.5 \cdot 10^{-4} m^2/s^2 \) to \( k = 2.5 \cdot 10^{-3} m^2/s^2 \), yields a larger mixing-layer growth rate than under base case conditions. The same observation can be made for the spreading rate of product mass fraction if compared to the base case. Free stream values of density, temperature and axial velocity remain unchanged. Maxima of the nondimensional axial velocity are 15% (at \( x = 50 \) mm) - 30% (at \( x = 12.5 \) mm) larger than the base case values. At \( x = 50 \) mm the maximum in \( \bar{u}(y)/u_{\infty} \) has shifted by about 0.3 mm towards the air side. The same shift is also observed for the minimum density value at that \( x \)-location. The minimum in \( \bar{\rho}(y) \) at \( x = 12.5 \) mm is slightly lower than in the base case; further downstream it has approximately the same values as in the base case.

In contrast to the base case, and to case 9, the transverse temperature profiles between \( x = 12.5 \) mm and \( x = 30 \) mm no longer have a common \( y \) location where all the profiles \( T(y) \) cross the same temperature value. At \( x = 12.5 \) mm the temperature maxima has shifted by 0.13 mm towards the air side, and at \( x = 50 \) mm, the shift is about 0.3 mm. This is consistent with the increase of the flame angle at \( x = 40 \) mm from 1.5° (in the base case) to 1.69° (see Table 1). Maximum temperature values are approximately the same as in the base case. Maximum values for the \( k(y) \) profiles between \( x = 12.5 \) mm and \( 50 \) mm are 11% (at \( x = 50 \) mm) - 30% (at \( x = 12.5 \) mm) larger than in the base case. As in the base case, the maxima are slightly shifted towards the fuel side. At \( x = 12.5 \) mm, the spreading of \( k \) is about 25% larger than for the base case (see Fig. 38). Between \( x = 12.5 \) mm and \( 50 \) mm, maximum \( \omega \)-values are between 20% (at \( x = 50 \) mm) and 30% (at \( x = 12.5 \) mm) smaller than in the base case (see Fig. 39).

The prescribed shift in the maxima values for density, temperature and axial velocity is also observed for the maximum mass fraction of products. According to the increased growth of the mixing layer, mass fraction of \( N_2 \) and product mass fraction on the fuel side and mass fraction of \( CH_4 \) on the air side are larger than in the base case. Gradients for all mass fractions at \( x = 50 \) mm are smaller than predicted for the base case. Contour plots of temperature and density for this case are illustrated in Figs. 40 and 41.

Free Stream Turbulent Specific Dissipation Rate; Growth of the mixing-layer is significantly increased in case 11 by the prescribed decrease in the free stream value of \( \omega \) from 500 s\(^{-1}\) to 5 s\(^{-1}\). At \( x = 12.5 \) mm, spreading of the velocity defect on the air side is 4.5 times the base case value, on the fuel side spreading is found to be 3 times the corresponding base case value. The spreading rate of product mass fraction is about 2.7 times larger than in the base case (see Table 2).

At \( x = 12.5 \) mm, the maximum of the nondimensional axial velocity component is 1.5 times its base case value, with a shift of 0.35 mm towards the air side. The same spreading as observed for the velocity defect, is also observed for the density defect. The minimum in the density profile \( \bar{\rho}(y) \) at \( x = 12.5 \) mm is only slightly lower than the base case value, but (analogous to the location of the velocity maximum) shifted about 0.35 mm towards the air side. The maximum temperature at \( x = 12.5 \) mm is the same as in the base case, but shifted analogous to the prescribed re-location of the density minimum and the
velocity maximum at that x-position. Contour plots for temperature, turbulent kinetic energy and specific dissipation rate \( \omega \) are illustrated in Figs. 42, 43 and 44. The maximum \( k \)-value at \( x = 12.5 \text{ mm} \) is about 50 \% larger than in the base case, whereas the corresponding maximum of \( \omega \) is 70 \% smaller than for the base case. Note that the axial flame stand-off distance and the ignition length are about half of those for the base case, whereas the flame stand-off in the y-direction is about twice the distance found in the base case. Also, one observes a significant increase of the flame angle to approximately 2.4\(^\circ\). A contour plot for the mass fraction of oxygen is shown in Fig. 45. Comparison of Fig. 45 with other cases (e.g. Fig. 27), suggests that oxygen mass fraction on the fuel side will be larger for larger flame-standoff distances \( x_{fl} \) and \( y_{fl} \). The latter allowing for increased transfer of \( \text{O}_2 \) to the fuel side before the flame is established. Note that, in the prescribed case the mixing layer has already reached the boundaries of the computational domain after \( x = 20 \text{ mm} \).

The significant impact of the specific dissipation rate \( \omega \) in the free stream on the growth of the free mixing layer has already been described by Wilcox.\(^{34}\) However, the increase in spreading rate with decreasing free stream \( \omega \) value observed here is significantly larger than the increase predicted in Ref. 24 for the non-reacting single-component mixing layer configuration. In the second edition of his book, Wilcox proposes a modification in the coefficients \( \beta^* \) and \( \beta \) (see Eqs. 15, 16), which, as reported, provides better agreement with experimental measurements for mixing layers and which reduces the prescribed sensitivity of the \( k-\omega \) model on the free stream values of \( \omega \).

In case 12, the growth of the mixing layer is smaller than predicted for the base case configuration. Spreading of the velocity defect at \( x = 37.5 \text{ mm} \) is reduced by about 25 \% on the air side and 30 \% on the fuel side (see Fig. 46). Maximum nondimensional velocity values at \( x = 25, 37.5 \text{ and } 50 \text{ mm} \) are reduced by approximately 20 \% from their base case values. At \( x = 12.5 \text{ mm} \), the maximum nondimensional velocity is only slightly larger than the nondimensional free stream air velocity. Note that the predicted flame stand-off distance in this case is 13 mm (see Table 1). In the base case \((u_{\text{max}} - u_{\infty})/u_{\infty} \) is approximately 0.06. Minimas of transverse density profiles at \( x = 25 \text{ mm} \) and higher are approximately the same as in the base case; however, they are slightly shifted away from the air side towards \( y = 0 \text{ mm} \). At \( x = 12.5 \text{ mm} \), \( \rho_{\infty} - \rho_{\text{min}} \) is about half the value predicted in the base case. Maximum temperature values at \( x = 25, 37.5 \text{ and } 50 \text{ mm} \) are approximately the same as in the base case, however, at \( x = 12.5 \text{ mm} \) \((T_{\text{max}} - T_{\infty})/T_{\infty} \) is just one third of the value observed in the base case. Again this is due to the larger flame stand-off distance in this case. Spreading of the temperature profile at \( x = 37.5 \text{ mm} \) is about 70 \% of the value found for the base case. The flame angle is is about 20 \% smaller than in the base case and the spreading rate of product mass fraction is reduced by 34 \% (see Fig. 47 and Table 2).

Contour plots for \( k \) and \( \omega \) are shown in Figs. 48 and 49. Maximum \( k \)-values are slightly shifted towards the air side \((y > 0 \text{ mm})\); in the base case maximum \( k \)-values are found at \( y < 0 \text{ mm} \). Maximas in \( k(y) \) are 50 \% \((x = 12.5 \text{ mm})\) or 85 \% \((x = 50 \text{ mm})\) of the values found in the base case. At \( x = 12.5 \text{ mm} \), the maximum \( \omega \)-value is a little larger than its base case counterpart, i.e. 2 times its free stream value. At \( x = 50 \text{ mm} \), the maximum in \( \omega \) is about 20 \% larger than in the base case.

At \( x = 50 \text{ mm} \), maximum product mass fraction is the same as in the base case. As mentioned earlier, this is true for all cases 0 - 12. This maximum location is shifted about 0.2 \text{ mm} towards the \( y = 0 \text{ mm} \) line. Gradients of the different species mass fractions are larger within the mixing layer at \( x = 50 \text{ mm} \). The mass fraction of oxygen at \( x = 50 \text{ mm} \) is about 0.01, whereas in the base case it is only half of that. A contour plot for the mass fraction of \( \text{O}_2 \) is provided in Fig. 50.

In order to complement the above discussion, to allow comparison among the different cases and to provide some basic characteristics of the diffusion flames, Tables 1 and 2 provide ignition lengths \( x_{ig} \), flame stand-off distances \( x_{fl} \) and \( y_{fl} \), flame angle as well as the spreading rates for the product mass fraction on both fuel and air sides, i.e. \( sr_{fuel} \) and \( sr_{air} \). Here, ignition length, specifies the distance between the splitter plate and the axial location, where the first local maximum in temperature is observed. Ignition lengths reported in Table 1 and put in parentheses indicate that, prior to ignition at the denoted \( x \)-location, ignition was found at the splitter plate, followed by extinction. Note that, the employed grid size is at times only one order of magnitude smaller than the ignition length \( x_{ig} \) (cases with \( x_{ig} = 0 \text{ mm} \) excluded).

The flame-standoff distance \( x_{fl} \) measures the axial distance between the end of the splitter plate and the location where the temperature gradients are the largest in the flowfield. Similarly, \( y_{fl} \) denotes the distance of the point with the largest temperature gradient from the \( y = 0 \text{ mm} \) line. Spreading rates \( sr_{fuel,air} \) have been determined at \( x = 20 \text{ mm} \) or \( x = 40 \text{ mm} \) from the angles between the line of maximum product mass fraction and the contour line for a product mass fraction of \( 10^{-3} \). See Fig. 2.

**Conclusions**

An accelerating turbulent reacting mixing layer of methane and air has been studied. The turbulent boundary-layer equations were solved numerically by
assuming a one-step chemical reaction mechanism and by using a \( k-\omega \) model to describe turbulence effects. The employed two-equation turbulence model has been benchmarked for the non-reacting single-component mixing-layer configuration. For the turbulent reacting case, spreading of the transverse velocity and temperature profiles at \( x = 12.5 \text{ mm} \) downstream from the splitter plate is about 5 times larger on the air side, and 12 times larger on the fuel side, in comparison to the laminar case. At \( x = 37.5 \text{ mm} \) these factors are 15 and 23, respectively. Parametric studies on the effect of changes in initial air temperature, pressure gradient, air stream velocity and fuel stream velocity have been carried out by varying each of these quantities separately by a maximum of \( 18 \% , 75 \% , 50 \% \) and \( 80 \% \), respectively. The resulting maximum changes in ignition length and axial flame stand-off distance are approximately \( 100 \% \) and \( 80 \% \), respectively. Sensitivity of the employed turbulence model to free stream values of \( k \) and \( \omega \) has been analyzed. Variations of the free stream value of \( k \) by two orders of magnitude were found to cause a maximum change in the ignition length by \( 20 \% \) and a maximum change in the axial flame stand-off distance by \( 50 \% \). More dramatic changes where found for variations of the free stream specific dissipation rate \( \omega \). Here, variation of \( \omega \) in the free stream by two orders of magnitude resulted in a maximum change of \( 220 \% \) in ignition length and a maximum change of \( 85 \% \) in the axial flame stand-off distance.

Acknowledgments
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References
### Table 1  Parameter survey and results for ignition length $x_{ig}$, axial flame stand-off distance $x_{fl}$, transverse flame stand-off distance $y_{fl}$, and flame angle. Flame angle evaluation at $x = 20 \text{ mm}$ (denoted by '*) or $x = 40 \text{ mm}$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$T_{air}$ [K]</th>
<th>$dp/dx$ [N/m$^2$]</th>
<th>$u_{air}$ [m/s]</th>
<th>$u_{fuel}$ [m/s]</th>
<th>$k$ [m$^2$/s$^2$]</th>
<th>$\omega$ [s$^{-1}$]</th>
<th>$x_{ig}$ mm</th>
<th>$x_{fl}$ mm</th>
<th>$y_{fl}$ mm</th>
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<td>500</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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<td>-50</td>
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<td>(4.8)</td>
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<td>1.21</td>
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### Table 2  Spreading rates of product mass fraction $sr = \arctan \theta$, where $\theta$ is the spreading angle on the fuel (index: fuel) or air side (index: air) based on the $10^{-3}$-contour line. $sr_{tot} = sr_{air} + sr_{fuel}$. Spreading rate evaluation at $x = 20 \text{ mm}$ (denoted by '*) or $x = 40 \text{ mm}$.

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<th>$sr_{tot}$</th>
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<td>0.080</td>
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<td>0.018</td>
<td>0.061</td>
<td>0.079</td>
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Fig. 1 Comparison with experimental\textsuperscript{27} and numerical results\textsuperscript{24} for a non-reacting single-component mixing layer, with zero velocity on one side of the splitter plate.

Fig. 2 Configuration under investigation. Definition of geometric flame parameters.

Fig. 3 Nondimensional axial velocity profiles for a reacting laminar (solid) and turbulent (broken lines) mixing layer. Laminar solutions are at $x = 12.5, 37.5$ mm, turbulent solutions (i.e. for case 0) are at $x = 12.5$ mm (dotted), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed).

Fig. 4 Temperature profiles for a reacting laminar (solid) and turbulent (broken lines) mixing layer. Laminar solutions are at $x = 12.5, 37.5$ mm, turbulent solutions (i.e. for case 0) are at $x = 12.5$ mm (dotted), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed).
Fig. 5  Density profiles for a reacting laminar (solid) and turbulent (broken lines) mixing layer. Laminar solutions are at $x = 12.5, 37.5$ mm, turbulent solutions (i.e. for case 0) are at $x = 12.5$ mm (dotted), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed).

Fig. 6  Species mass fractions versus $y$ at $x = 50$ mm for case 0 (the base case).

Fig. 7  Temperature contours for case 0 (the base case).

Fig. 8  Temperature contours for case 0 (the base case) near the ignition point.
Fig. 9 Velocity profiles versus $y$ for case 0 (the base case) at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (dotted) and $x = 50$ mm (dot-dashed).

Fig. 10 Contour lines of oxygen mass fraction for case 0 (the base case).

Fig. 11 Contour lines of $k$ for case 0 (the base case).

Fig. 12 Contour lines of $\omega$ for case 0 (the base case).
Fig. 13  Mach number profiles versus $y$ for case 0 (the base case) at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (dotted) and $x = 50$ mm (dot-dashed).

Fig. 14  Mach number contour lines for case 0 (the base case).

Fig. 15  Contour lines of product mass fraction (i.e. CO$_2$ and H$_2$O) for case 0 (the base case).

Fig. 16  Velocity profiles versus $y$ for case 1 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.
Fig. 17  Temperature profiles versus y for case 1 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 18  Contour lines of $k$ for case 1.

Fig. 19  Species mass fractions versus y at $x = 50$ mm for case 1.

Fig. 20  Density profiles versus y for case 2 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.
Fig. 21  Temperature contours for case 2.

Fig. 22  Density profiles versus $y$ for case 3 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 23  Temperature profiles versus $y$ for case 3 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 24  Turbulent kinetic energy profiles versus $y$ for case 3 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.
Fig. 25  Temperature contours for case 4.

Fig. 26  Contour lines of \( k \) for case 4.

Fig. 27  Contour lines of oxygen mass fraction for case 4.

Fig. 28  Species mass fractions versus \( y \) at \( x = 20 \) mm for case 4.
Fig. 29  Contour lines of $k$ for case 5.

Fig. 30  Contour lines of $\omega$ for case 5.

Fig. 31  Axial velocity contours for case 6.

Fig. 32  Species mass fractions versus $y$ at $x = 50$ mm for case 6.
Fig. 33 Temperature contours for case 7.

Fig. 34 Species mass fractions versus $y$ at $x = 20$ mm for case 7.

Fig. 35 Velocity profiles versus $y$ for case 8 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 36 Density profiles versus $y$ for case 8 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.
Fig. 37  Temperature profiles versus \( y \) for case 9 at \( x = 12.5 \) mm (solid), \( x = 25 \) mm (dashed), \( x = 37.5 \) mm (long dashed) and \( x = 50 \) mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 38  Turbulent kinetic energy profiles versus \( y \) for case 10 at \( x = 12.5 \) mm (solid), \( x = 25 \) mm (dashed), \( x = 37.5 \) mm (long dashed) and \( x = 50 \) mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 39  Profiles of the specific dissipation rate \( \omega \) versus \( y \) for case 10 at \( x = 12.5 \) mm (solid), \( x = 25 \) mm (dashed), \( x = 37.5 \) mm (long dashed) and \( x = 50 \) mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 40  Temperature contours for case 10.
Fig. 41  Density contours for case 10.

Fig. 43  Contour lines of $k$ for case 11.

Fig. 42  Temperature contours for case 11.

Fig. 44  Contour lines of $\omega$ for case 11.
Fig. 45 Contour lines of oxygen mass fraction for case 11.

Fig. 46 Velocity profiles versus y for case 12 at $x = 12.5$ mm (solid), $x = 25$ mm (dashed), $x = 37.5$ mm (long dashed) and $x = 50$ mm (dot-dashed). Dotted lines are the corresponding base case profiles.

Fig. 47 Contour lines of product mass fraction (i.e. CO$_2$ and H$_2$O) for case 12.

Fig. 48 Contour lines of $k$ for case 12.
Fig. 49  Contour lines of $\omega$ for case 12.

Fig. 50  Contour lines of oxygen mass fraction for case 12.