AN EFFICIENT COMPUTATIONAL MODEL FOR PREMIXED TURBULENT COMBUSTION AT HIGH REYNOLDS NUMBERS BASED ON A TURBULENT FLAME SPEED CLOSURE

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ABSTRACT
Theoretical background, details of implementation and validation results of a computational model for turbulent premixed gaseous combustion at high turbulent Reynolds numbers are presented. The model describes the combustion process in terms of a single transport equation for a progress variable; closure of the progress variable's source term is based on a model for the turbulent flame speed. The latter is identified as a parameter of prime significance in premixed turbulent combustion and is determined from theoretical considerations and scaling arguments, taking into account physico-chemical properties of the combustible mixture and local turbulent parameters. Specifically, phenomena like thickening, wrinkling and straining of the flame front by the turbulent velocity field are considered, yielding a closed form expression for the turbulent flame speed that involves, e.g., speed, thickness and critical gradient of a laminar flame, local turbulent length scale and fluctuation intensity. This closure approach is very efficient and elegant, as it requires only one transport equation more than the non-reacting flow case, and there is no need for costly evaluation of chemical source terms or integration over probability density functions.

The model was implemented in a finite-volume based computational fluid dynamics code and validated against detailed experimental data taken from a large scale atmospheric gas turbine burner test stand. The predictions of the model compare well with the available experimental results. It has been observed that the model is significantly more robust and computationally efficient than other combustion models. This attribute makes the model particularly interesting for applications to large 3D problems in complicated geometries.

NOMENCLATURE
- \( \rho \) Density
- \( T \) Temperature
- \( c \) Progress variable
- \( a \) Rate of strain
- \( \sigma \) Critical strain rate
- \( G \) Stretch Factor
- \( U_l, \delta_l \) Laminar flame speed and thickness
- \( U_{nt}, \delta_{nt} \) Thickened flame speed and thickness
- \( k \) Turbulent kinetic energy
- \( \epsilon \) Turbulent dissipation rate
- \( \nu' \) Turbulent velocity
- \( l_t \) Turbulent integral length scale
- \( \tau_t \) Turbulent turnover time
- \( \tau_c \) Chemical heat release time
- \( Re \) Turbulent Reynolds number
- \( Da \) Damköhler number
- \( Sc \) Schmidt number
- \( \nu, \nu_t \) Dynamic, turbulent viscosity
- \( \chi \) Molecular heat transfer coefficient
- \( \lambda \) Excess air ratio

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INTRODUCTION

The lean-premixed technique has proven very successful in reducing emissions of NO\textsubscript{x} from gas turbines and has – at least for gaseous fuels – established itself as a standard for modern utility gas turbines. However, the designer of a lean-premixed gas turbine combustor is confronted with challenging difficulties which are either unique to the lean-premixed mode of combustion, or which are less severe in more conventional diffusion flame combustors. These difficulties are – to name but the most prominent ones – flame flash-back, lean blow-out, excessive emissions of CO, thermoacoustic instabilities and the detrimental effect of imperfect fuel-air mixing on pollutant emissions and combustion stability.

If numerical modeling is to make a useful contribution to lean-premixed gas turbine design, the quantitatively correct prediction of the average rate of heat release is of utmost importance, as this parameter controls directly flame flash-back and blow-out. Furthermore, modeling mean heat release correctly is a prerequisite for the prediction of practically all other phenomena of interest.

In this report theoretical background, implementation and validation of a turbulent combustion model suitable for lean-premixed gas turbine applications with high Reynolds numbers and moderately fast chemistry are described. The model is formulated in terms of a single transport equation for a progress variable, which can – in its basic form – be used for numerical modeling of the average rates of heat release and products creation. The closure for the progress variable's source term is based on a model for the turbulent flame speed, which is considered to be the main hydrodynamic and physico-chemical parameter of premixed turbulent combustion. The following physico-chemical phenomena are considered in the determination of this velocity:

- Influence of fuel concentration, fuel composition and pressure on the combustion process.
- Thickening and distortion of the flame front by small-scale and large-scale turbulence at high turbulent Reynolds number Re and moderate Damköhler number Da.
- Quenching by turbulent straining ("stretch effect").
- Changes of local composition in regions of high turbulent strain due to the different molecular diffusivities of heavy and light species ("preferential diffusion effect").

Theoretical considerations, scaling arguments, numerical simulations of laminar flames and experimental data are combined to eventually yield analytical, "closed form" expressions for the diffusion and source terms in the transport equation for the progress variable. We emphasize that the popular "fast chemistry" assumption, which is arguably not adequate for lean-premixed combustion at gas turbine conditions, is not invoked.

In previous publications [1, 2, 3, 4] the model was validated against standard experimental data on turbulent flame speeds and against propagation speeds of spherical combustion waves in stirred bombs for different fuels, stoichiometric ratios and turbulent velocities. In this work, the model was implemented in a three-dimensional computational fluid dynamics code and validated against detailed data from experiments at atmospheric pressure in a large scale gas turbine burner test stand.

The paper is organized as follows: the transport equation for the progress variable and its closure are described in the next Section. Then a model for the turbulent flame speed, required to complete the closure, and the "stretch effect" extension of the model, which is needed at high turbulent intensities, are introduced and discussed in some detail. The final Sections describe the experimental setup, the numerical implementation and results of 3D validation computations.

TURBULENT FLAME SPEED CLOSURE

In engineering calculations of premixed turbulent combustion, the chemical processes resulting in products creation and heat release can in many cases be described adequately with a single progress variable c. It is defined here as a normalized mass fraction of products (c=0 in the unburnt mixture and c=1 in the products). The (unclosed) transport equation for c has the form [5]:

$$\frac{\partial}{\partial t} (\rho \bar{c}) + \frac{\partial}{\partial x_k} (\rho \bar{u}_k \bar{c}) = \frac{\partial}{\partial x_k} \left( \rho \frac{\partial c}{\partial x_k} \right) + \bar{w}_c.$$  \hspace{1cm} (1)

Both Reynolds averages (\ldots) and Favre averages (\ldots) are used with

$$\bar{p} \cdot \bar{c} = \bar{\rho} \bar{c},$$  \hspace{1cm} (2)

$$c'' = (c - \bar{c}).$$  \hspace{1cm} (3)

The transport equation (1) for c is closed by substituting

$$\bar{w}_c = \rho_c U_t |\nabla c|.$$  \hspace{1cm} (4)
for the source term, where \( U_t (>0) \) is a velocity scale dependent upon the physico-chemical characteristics of the combustible mixture and the local turbulence parameters. This Turbulent Flame Speed Closure (TFC) for the source term was proposed by Zimont [6]. It is related to the so-called G-equation\(^1\), first proposed by Markstein [7] for laminar flames and further developed by Peters and others (see the references in [8]) in the context of turbulent premixed combustion.

Some aspects of the closure ansatz (4) shall be illustrated briefly by considering the 1-D case. Assuming for the moment stagnating medium \( (u_t = 0) \), fixed turbulence parameters and density (in this case \( U_t = \text{const} \) and \( \nu_t = \text{const} \)), the transport equation for \( c \) can be written as

\[
\frac{\partial c}{\partial t} = \frac{\nu_t}{\rho_{uc}} \frac{\partial^2 c}{\partial x^2} + U_t \frac{\partial c}{\partial x}.
\]  

(5)

Clearly, equation (5) describes a "combustion" wave moving with velocity \( U_t \) from right to left. Furthermore, the width of the wave is growing due to turbulent diffusion\(^2\).

Note that (4) contains the unburnt mixture density \( \rho_u \) because only then equations (1) and (4) result in the correct reactant flow rate, which is equal to \( \rho_u U_t \) for constant \( U_t \) (this can be proved rigorously). Then integration of (5) between \( x = -\infty \) to \( x = +\infty \) (in a coordinate system moving with velocity \( U_t \)) leads to the mass conservation equation

\[
\rho_u (\bar{u}_b + U_t) = \rho_u U_t.
\]  

(6)

Temperature can be computed directly from the reaction progress variable \( c \) as

\[
T(c) = (1-c)T_u + cT_b,
\]  

(7)

where the indexes \( u \) and \( b \) denote the unburnt and burnt values. Density \( \rho \) is then easily found using the gas law, assuming constant pressure and constant mean molecular weight.

A MODEL FOR \( U_t \)

Obviously a model for the turbulent flame speed \( U_t \) is needed in order to make the closure (4) complete. In a first step, the model developed by Zimont [6] (see also Borghi [9]) for wrinkled and thickened flamelets\(^3\) is used to express \( U_t \) in terms of turbulence parameters and physico-chemical characteristics of the combustible mixture.

We will now present a short overview of this model, in order to better illustrate its applicability and limitations. The core idea is that small-scale turbulent structures intensify the transfer processes inside the flamelets and determine their thickness \( \delta_{nt} \) and propagation velocity \( U_{nt} \), while large-scale turbulent vortices wrinkle the "thickened" flamelets and control the width of the averaged turbulent combustion zone. The total flamelet area depends on the entire spectrum of turbulence and is determined by its integral characteristics and by the parameters of the thickened flamelets. This mechanism of turbulent combustion is only possible, if there is a physical mechanism able to limit the expansion of the thickened flamelets. It has been shown [6, 9, 12] that larger and larger vortices are engulfed by the thickened flamelets, until an equilibrium is established between convection, heat conduction and chemical reaction processes. The following relations

\[
U_{nt} \sim u'Da^{-1/2} > U_t, \\
\delta_{nt} \sim l_t Da^{-3/2} > \delta_t,
\]

(8)

have been derived, using dimensional analysis\(^4\) and Kolmogorv scaling for small-scale turbulence.

The average turbulent flame velocity \( U_t \) is larger than the velocity of the "thickened" front \( U_{nt} \) by a factor which depends on the ratio between the area \( \delta S \) of a flame surface element and the projection \( \delta S_0 \) of this element normal to the direction of average flame front propagation:

\[
U_t \sim \frac{U_{nt} \delta S}{\delta S_0},
\]

(9)

where \( \Sigma^2 = (z - \bar{z})^2 \) is the variance in flame position due to turbulent convection \( z = z(x, y) \) is local position of the flamelet element), and \( \Lambda \) denotes the microscale of the random flame front surface.

For the purpose of estimating \( \Sigma \), and provided that \( U_{nt} \ll u' \), the combustion front can be considered to consist approximately of the same fluid particles. Con-

\(^1\)not to be confused with the the "stretch factor" \( C \), see below

\(^2\)This is apparent if the 1-D transport equation (5) for \( c \) is expressed in a coordinate system \( x' = x + U_t t \) moving with the front, then (5) reduces to the standard diffusion equation.

\(^3\)It is generally agreed that wrinkled and thickened flame structures are characteristic for lean-premixed gas turbine combustion, due to the high turbulent intensities and relatively long chemical times prevalent at these conditions, see e.g. Polilke et al. [10], Sattelmayer et al. [11].

\(^4\)Recall that \( Da \sim \tau_t/\tau_c \gamma_t \sim \tau_t/u'; \tau_c \sim \chi_c/U_t^2 \).
sequently, $\Sigma^2$ is subject to the customary turbulent diffusion relationship

$$\Sigma^2 \sim D_t t \sim u' l_t t,$$

(10)

where $D_t$ is a constant turbulent diffusion coefficient and the time $t$ is in the range

$$\tau_1 \leq t \ll \frac{l_t}{U_{nt}} \sim \tau_t D_a^{3/2}.$$

(11)


In a statistically stationary situation,

$$\Lambda \sim (u' \delta_{nt})^{1/2}$$

(12)

follows from the requirement that $U_t$ be constant and dimensional considerations. Combining (8), (10) and (12), we obtain

$$\left(\frac{\delta S}{\delta S_0}\right) \sim \left(\frac{l_t}{\delta_{nt}}\right)^{1/2} \sim D a^{3/4},$$

(13)

which yields combined with (8) and (9) finally an expression for the turbulent combustion velocity:

$$U_t = A u' \frac{1}{2} U_t^{1/2} x_u^{1/2} l_t^{3/4}. $$

(14)

The molecular heat transfer coefficient of the unburnt mixture $x_u$ can be found in standard references or determined with suitable computer programs. Similarly, laminar flame speeds $U_l$ for many fuels and operating conditions of interest can be found in the literature or can be determined in experiments or with computations of 1D laminar flames with a detailed chemical mechanism. Note that changes in pressure, fuel concentration, etc. will affect the parameters $x_u$ and $U_l$ and thereby influence the value of $U_t$ in a well-defined and physically meaningful way.

Assuming that a standard $k - \epsilon$ turbulence model is used, values for turbulent intensity $u'$ and length scale $l_t$ can be obtained from turbulent kinetic energy $k$ and dissipation $\epsilon$. The prefactor $A$ has been determined by evaluation of a large experimental database of stirred bomb experiments in [2, 3]. The value $A = 0.52$ reproduces experimentally found turbulent flame speeds for a wide range of fuels and operating conditions with good accuracy. Herewith complete closure for the progress variable’s source term has been achieved. Note that all parameters appearing on the l.h.s of (14) are one of the following a) overall numerical constants b) constants describing physico-chemical properties of the combustible mixture or c) readily derived from a standard two-equation turbulence model.

It is worth emphasizing that (14) has been rigorously derived from the underlying physical model and dimensional analysis and does not contain empirical information with the exception of the constant $A$ (which should be of order unity). This "rigid" theoretical construction allows to reduce to a minimum the number of empirical parameters (used for "tuning" the combustion model) and assures fixed dependence on controlling factors.

The relations (8) and (14) are valid if

$$Re^{3/4} D_a^{-3/2} > 1 > D a^{-1/2}.$$  

(15)

It can be shown from this relation that the combustion model applies when vortices of minimal scale (Kolmogorov length) are smaller than the width of the laminar flame. For insufficiently large $Re$ the flamelets will be laminar, for large $\tau_t$ (small $Da$) $U_{nt}$ will be of the order of $u'$ and wrinkling of flamelets will not occur.

The various powers in (14) expressing the dependence of $U_t$ on the physico-chemical and turbulent properties of the combustible mixture are in good agreement with experimental results, the interested reader is referred to [1, 2, 3, 4].

Equation (14) does not take into account two physical effects which are significant under certain circumstances: preferential diffusion and turbulent "strain". The latter effect provides an explanation for the experimentally observed reduction in turbulent combustion intensity at very high turbulent velocities and is connected with the straining of flamelets by small-scale turbulent eddies. This "stretch effect" is of importance for low-emission gas turbines and indeed should be incorporated in any combustion model designed for high turbulent Reynolds numbers, particularly if combustion near lean blow-off is considered – see the next section.

Preferential diffusion, on the other hand, causes local composition changes in the distorted and strained flamelets, due to different molecular diffusion coefficients of fuel and oxidizer. Consequently, maximum turbulent combustion rates are achieved with slightly lean mixtures for light fuels (like hydrogen, methane) and slightly rich mixtures for heavy fuels (like propane, vaporized oil), respectively. This effect has also been introduced in the model. However, as it is of only minor importance if methane or natural gas is used as fuel, no details are given in this report and the interested reader is referred to [2, 3].

In concluding this Section, we want to point out that the model for turbulent flame speed just presented is particularly suitable for the case of lean-premixed combustion in gas turbines. Specifically, the extremely high
turbulent Reynolds \( \text{Re} \) numbers prevalent in gas turbines, and the relatively large chemical time scales typical of fuel lean combustion ensure that relations (15) — which govern the applicability of the model (14) for turbulent flames speeds — are satisfied. We emphasize again that changes in operating pressure, inlet temperature, fuel concentration and fuel composition\(^5\) affect the predicted value of turbulent flame speed \( U_f \) in a well-defined and physically meaningful way.

THE STRETCH EFFECT

As mentioned above, for industrial low-emission combustors operated near lean blow-off the effect of strain or "stretch" must have a considerable impact on the mean turbulent heat release intensity. To expand the range in which the proposed closure may be used, we have combined it with the model of flamelets quenching through stretching suggested by Bray [13]. Differently strained flamelets are reduced to either unstrained ones (no quenching) if the absolute value \( g \) of the velocity gradient is less than some critical value \( g_{cr} \), or to highly strained flamelets (with negligible contribution to the reaction progress) for \( g > g_{cr} \).

To take the stretch effect into account, the source term (4) of the progress variable equation is multiplied by a stretch factor \( G \) — the probability of unquenched flamelets — which is obtained by integrating the lognormal distribution\(^6\) of the turbulent dissipation rate \( \varepsilon \)

\[
G = \frac{1}{2} \text{erfc} \left\{ -\frac{1}{2\sigma} \left( \frac{\varepsilon - \mu_{\varepsilon}}{\sigma_{\varepsilon}} + \frac{\sigma}{2} \right) \right\},
\]

where \( \text{erfc} \) denotes the complementary error function and \( \sigma = \mu_{\varepsilon} \ln (L/\eta) \) is the standard deviation of the distribution of \( \varepsilon \), with \( \mu_{\varepsilon} \) a constant measured to be 0.26 and \( \varepsilon_{cr} = 15\mu_{\varepsilon}^2 \).

For steady laminar flows the critical velocity gradient \( g_{cr} \) for flame quenching may be obtained numerically, see for example Rogg [14]. But difficulties emerge in using these results for the present purpose. Different stationary model problems (single-flame or twin-flame configuration) give large variations in the predicted variations of \( g_{cr} \). Additionally, in turbulent flows \( g_{cr} \) must be larger than in the stationary cases, as the smallest turbulent eddies (resulting in the largest strain rates) do not persist long enough to quench a flame front locally. For this reason the values of \( g_{cr} \) to be used in industrial simulations have to be tuned and theory or numerical modeling can only suggest a range of physically plausible values. Indeed, \( g_{cr} \) is the only significant parameter for "tuning" the TFC model to the DCB experimental data.

MODEL VALIDATION

Previous model validation has been focused on: a) a comparison of the expression (14) for the turbulent flame velocity with experimental data on premixed turbulent combustion [2, 3, 4]; b) a comparison of the calculated consumption rate in spherical premixed turbulent flames using (1) and (4) with direct experimental measurements in stirred bombs [2], using different fuels \( (\text{CH}_4, \text{C}_2\text{H}_6, \text{C}_3\text{H}_8, \text{H}_2) \) and different air excess ratios (typically in the range 0.6 - 1.6).

In general, good agreement between the TFC model and experimental data has been observed. As already mentioned above, it was found that \( A = 0.52 \) is the optimum value for the hydrocarbon fuels investigated and \( A = 0.61 \) for hydrogen (though the results obtained using \( A = 0.52 \) were quite satisfactory also for hydrogen).

In the present work, the TFC model has been validated against detailed experimental data from an ABB Double Cone Burner (DCB) with 0.17 m nominal diameter mounted in an atmospheric test rig. A DCB comprises two halves of a cone that are shifted with respect to each other in the radial direction such that two inlet slits of constant width are formed. A strong tangential component is imparted to the gas entering the burner through these slits. The degree of swirl is chosen such that at the burner outlet the flow undergoes a vortex breakdown, resulting in a zone of recirculation, which acts as an aerodynamic flame holder. This type of flame stabilization in free space is the characteristic property of the DCB. Fuel gas is injected through a number of small holes along the burner's inlet slits, providing a high degree of fuel-air premixing and making flame flashback into regions upstream of the burner impossible. More details have been given by Sattelmayer et al. [15].

The burner used in the experiments fires into a ceramically insulated combustion chamber of square cross section with 0.28 m side length, see Fig. (1). For the experiments reported here, the burner is operated with a mass flow rate of about 0.3 kg/s. Using natural gas as fuel at an excess ratio \( \lambda = 2 \) and pre-heating the combustion air with an electrical heater such that the inlet temperature of the combustible mixture \( T_i = 650 \text{ K} \), an
adiabatic temperature $T_{ad} \approx 1755$ K is reached. The stability of the operation point during the experiments is maintained by controlling the global excess ratio calculated from an exhaust gas sample taken at the far end of the combustion chamber. The variations in $\lambda$ do not exceed ±0.01.

With an estimated turbulent length scale $l_t \approx 0.005$ m and turbulent intensities of order $u' \approx 10$ m/s (as observed in experiment), the DCB's turbulent Reynolds number is of order 1000, which is certainly higher than typically reached in laboratory-scale experiments. At the lean conditions considered here, chemical time scales are quite large, and one may estimate the Damköhler number $Da \approx 3$. This suggests quite significant flamelet thickening through turbulent transport; the relation (15), which determines the applicability of the TFC model is just barely fulfilled. Indeed, (8) yields $\delta_{nu} \approx 0.5 l_t$.

Diagnostic access is provided such that measurements of temperature, chemical species and velocities can be performed in the streamwise horizontal and vertical planes as well as in the axis-normal plane at various downstream positions and with up to several hundred positions per measurement plane. An uncoated Pt – PtRh thermocouple, mounted on an uncooled ceramic probe, is used to measure temperature. No corrections for radiation loss are made, as too many of the relevant parameters needed for an exact radiation correction are not known. The maximum errors in temperature measurement are estimated to less than 70 K. Mean and fluctuating values of the axial component of velocity were determined with Laser-Doppler anemometry (LDA). Note that the measurement results shown in the following Figures represent temporal mean values, averaged over 10 s per data point.

**NUMERICAL IMPLEMENTATION**

The geometry of the DCB, the combustion chamber and the upstream plenum was represented by a boundary-fitted, structured, single-block computational grid with approximately 230,000 computational cells. This resolution is not enough to resolve fuel-injection along the slits with sufficient accuracy. Therefore in the computations, homogeneous fuel-air mixture enters the inlet section of the computational domain, i.e. the upstream side of the plenum.

Implementation of the basic TFC model (see Eqns. (1) and (4)) in a finite volume based fluid dynamics code that relies on the well-known $k - \varepsilon$ model [16] for the computation of turbulent flows has proven to be straightforward, as the transport equation for $c$ is in standard form. The heat release sub-model couples with the flow field only via the density $\rho$, which can be computed from the progress variable $c$ as follows:

$$\frac{1}{\rho(c)} = \frac{1-c}{\rho_u} + \frac{c}{\rho_b},$$

assuming constant pressure and mean molecular weight and invoking the standard definition of the progress variable. Again the indexes $u$ and $b$ refer to the unburnt and burnt state, respectively.

The turbulent intensity $u'$ and length $l_t$ were computed from turbulent kinetic $k$ and dissipation $\varepsilon$ using the standard constants of the $k - \varepsilon$ model as given in [16].

Some difficulties occurred with the computation of the source term $\overline{w_c}$, which requires knowledge of the gradient of the progress variable (see Eqn. (4)). Using a standard second order central difference scheme to compute the gradient of $c$ from its cell center values, it was observed that in regions where the computational grid is highly skewed and non-uniform, the gradient shows slight fluctuations which do not correspond to the $c$-field. It was investigated whether use of higher order schemes or a scheme based on Gauss' law would bring improvement in this respect. However, this was not the case, and the conclusion was that the TFC model should only be used on computational grids of good quality. Fortunately, these irregularities of the source term did not adversely affect the convergence behavior of the model, presumably due to the "smearing" effect.
of the diffusive term in the transport equation of the progress variable $c$. In general we have found that the TFC model is numerically benign and efficient.

Comparing the computational requirements of the TFC model against those of an extended Magnussen Model with two-step chemistry as used in [10] and a flamelet model ([17]) involving integrations of probability density functions for reaction progress and turbulent strain, we observe that the extended Magnussen model requires about two times and the flamelet model about four times as much CPU time per iteration as the TFC model. Also, we have experienced that the TFC model achieves convergence even if started from a very poor "initial guess", while especially the extended Magnussen model requires careful preparation of the initial flow, temperature and species concentration distributions if divergence of the iterative solution process is to be avoided.

RESULTS

An analysis of temperature and velocity distributions obtained with the TFC model shows that the qualitative features of the computed turbulent reacting flow field agree with design expectations [15], previous 2-D results [10] and the measurements. Most prominent is a central recirculation zone containing hot combustion products downstream of the burner exit, which acts as a hydrodynamic flame holder. Surrounding the central recirculation zone is an annular stream of fresh mixture displaying rather large axial velocities of more than twice the nominal burner exit velocity. In the corner formed by the front panel and combustor liner, there is an outer recirculation zone of smaller strength. The shear layers that separate the recirculation zones and the annular stream of fresh mixture provide intense turbulent mixing, heat release is highest in these regions.

A more careful comparison of experimental and computational results displays significant discrepancies between computation and experiment, in particular with respect to the size and location of the central recirculation zone, which is much too wide and too long in the computation. Also, the strength of the recirculation is significantly overpredicted. Profiles of axial velocity illustrating this observation are shown in Figs. 2 and 3.

In the experiment and to a lesser extent also in the computation, an asymmetry between the horizontal and the vertical planes of measurement was found, due to the imperfect axial symmetry of the burner (The burner's inlet slit are in the horizontal plane). Therefore, data from both planes of measurement are displayed in Figs. 2 - 5. Note that particularly in Figs. 2 and 5 the experimentally determined profiles of velocity in the two planes of measurement do not match at the intersection of the two planes, i.e. the centerline of the combustion chamber. This mismatch, which may help to assess roughly the accuracy of the experimental results, is in our opinion due to inaccuracies in probe positioning and alignment relative to the burner, and in the control of the operating point.

The deficiencies found are not necessarily a shortcoming of the TFC ansatz - strongly swirling flows are notoriously difficult to predict with $k-c$ and even Reynolds
Figure 4: Computed (—) vs measured (+) profiles of the progress variable $c$ at downstream position $z/D = 0.25$. Note that experimental data points from the left and right halves of the horizontal and the top and bottom halves of the vertical plane, respectively, have been overlayed in these graphs.

stress models. Indeed, a comparison of various turbulent combustion models carried out by Bettelini et al. [17] showed that the size and strength of the central recirculation zone was inadequately predicted with all combustion models considered. Clearly, the modelling of the turbulent exchange of momentum needs to be improved. Furthermore, although the grid employed in these simulations is certainly quite large, there is some evidence that the solutions obtained are not grid-independent, e.g. switching to higher order discretization schemes does have a noticeable influence on velocity and temperature fields. It is unfortunate that the interior of the burner is not accessible to measurements, as the details of the flow field inside the double cone would certainly provide valuable further insight into the intricacies of the flow field.

Profiles of the progress variable $c$ - which is essentially a normalized temperature - experiment and computation with the TFC model are compared in Figs. 4 and 5. Near the centerline computed temperature profiles are significantly higher then measured ones, clearly a consequence of the overpredicted convective transport of combustion products within the recirculation zone.

It is apparent that in the experiment, temperature distributions in the horizontal and vertical plane differ significantly from each other. Clearly, the present computation on the three-dimensional grid reproduces this asymmetry between vertical and horizontal planes only to some extent, resulting in elevated minimum values of the progress variable $c$ in the vertical plane, and delayed reaction in the horizontal plane. The overpredicted width and strength of the central recirculation zone, which is axisymmetric, is certainly to some extent responsible for the observed discrepancies in temperature distribution.

A value of $g_{cr} = 8000 \text{ s}^{-1}$ has been used for the computation presented here. Note that with a somewhat lower value, e.g. $g_{cr} = 6000 \text{ s}^{-1}$, the temperature increase at the axis occurs a bit further downstream (yielding better agreement with experiment in this respect), but then the off-axis regions of lower temperature extend too far downstream (not shown in Figures). These values for the critical gradient $g_{cr}$ correspond well with computations of quasi-1D strained laminar flames with detailed chemistry [14]: using the symmetrical (twin-flame) fresh-to-fresh configuration, extinction occurs at a strain rate $\alpha \approx 3000 \text{ s}^{-1}$, while for the asymmetrical fresh-to-burnt flame, an extinction strain rate $\alpha \approx 8000 \text{ s}^{-1}$ has been determined.

\footnote{The computational results shown were obtained with a second order upwind scheme and a $k-\varepsilon$ model with standard values for all model constants.}

\footnote{Again the experimentally determined profiles do not match exactly at the centerline.}

\footnote{Obviously, temperature cannot be used as an indicator of extinction for fresh-to-burnt flames, as the maximum temperature is always equal to the adiabatic temperature in this configuration. Also, the convergence behavior of the 1D laminar model does not indicate "extinction", as in our experience a converged solution can be obtained at all strain rates if one restarts from a previous solution with somewhat lower strain. We therefore define "extinction strain rate" for an fresh-to-burnt flame as the value $\alpha$ where the $OH$ concentration does not increase markedly above its equilibrium value throughout the computational domain. This criterion is physico-chemically well-motivated and works well for...}
In the present context, two "internal parameters" of the TFC model are of interest and plotted in Fig. 6: the stretch factor \( G \) (see Eqn. (16)) and the turbulent flame speed \( U_t \) (see Eqn. (14)). It is observed that in the shear layers surrounding the recirculation zone, \( G \approx 0.4 \), i.e., turbulent straining reduces combustion intensity by more than 50% in this region of the combustor. Also near the combustor walls the effect of the stretch factor is quite pronounced. The computed turbulent flame speed is quite non-uniform—reflecting the structure of the fields of turbulent kinetic energy \( k \) and dissipation \( \varepsilon \)—and peaks with 12 m/s at a value that is more than 20 times as large as the laminar flame speed for the conditions considered.

SUMMARY AND OUTLOOK

A model for premixed combustion at high Reynolds numbers that is based on a turbulent flame speed closure (TFC) has been implemented and validated with 3-D computations against detailed experimental data from a gas turbine burner test stand. The TFC model has performed satisfactory; qualitative features of the reacting flow have been well reproduced, and the model is computationally robust and very efficient. The latter fact is obviously of particular importance to industrial applications.

The TFC ansatz is in some sense quite similar to many combustion models that are currently in use in industry or investigated at a research level. In all these models, certain assumptions about the structure of the turbulent combustion process (e.g., the flamelet assumption) are made, and detailed sub-models are constructed to achieve closure for a particular equation. The rationale behind this approach is clearly that a combustion model will reproduce the correct dependence of the turbulent heat release rates or the width of the combustion front, etc., on the physico-chemical parameters, if all the sub-models involved describe the details of the turbulent combustion process with sufficient accuracy. Frequently, the sub-models are then solved numerically as part of the overall computation process, involving, e.g., integration over probability density functions and/or reduced chemical mechanisms, etc. Here is where the TFC model differs radically from its competitors, as established theoretical and experimental facts are introduced a priori in analytical form in the formulation of the model. This approach is not only computationally very efficient, as integration over probability density functions, determination of chemical reaction rates, etc., are not required; it also has the promise of reproducing "automatically" the experimentally observed influence of the main controlling factors on heat release intensity and temperature distributions. Whether the TFC model will fulfill this promise cannot be decided before parametric validation studies are carried out, covering, e.g., a range of equivalence ratios, pre-heat temperatures, Reynolds and Damköhler numbers, etc.

The TFC ansatz can be extended to the cases of partially premixed (see [18]) or non-adiabatic combustion. This work is in progress and shall be reported elsewhere. Also, exploiting the peculiarities of \( \text{NO}_x \) formation in lean-premixed combustion—as they are summarized, e.g., in [10, 11, 19]—it is relatively straightforward to construct a \( \text{NO}_x \) post-processor for the TFC model. This has already been done and good agreement with experiment has been achieved. Details shall be published elsewhere. Whether it is also possible to construct a "post-processor" for \( \text{CO} \) and unburnt hydrocarbons, or whether the TFC model can be extended to predict these emissions in some other way shall be the subject of future work.

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REFERENCES


