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Ramaekers, W.J.S.; Albrecht, B.A.; van Oijen, J.A.; de Goey, L.P.H.; Eggels, R.L.G.M.

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The application of Flamelet Generated Manifolds in modelling of turbulent partially-premixed flames

W.J.S. Ramaekers*, B.A. Albrecht, J.A. van Oijen and L.P.H. de Goey
Department of Mechanical Engineering
Eindhoven University of Technology, The Netherlands
R.G.L.M. Eggels
Rolls-Royce Deutschland Dahlewitz, Germany

Abstract
To reduce harmful emissions numerical models are developed to simulate combustion processes in engineering applications. In this paper a model for partially-premixed combustion used in Reynolds Averaged Navier-Stokes Simulations (RANS) is presented. A flamelet approach combined with a Probability Density Function (PDF) closure method for the chemical source term is used to describe turbulence-chemistry interaction. The laminar flamelet database is generated using the Flamelet Generated Manifold (FGM) chemistry reduction technique; it is assumed that mixing and chemistry are fully described by mixture fraction and a reaction progress variable respectively. A look-up database for turbulent combustion is constructed by PDF-averaging the laminar flamelet database. For the PDF a $\beta$-function is assumed. In this paper the FGM/PDF model as implemented in FLUENT is described and validated for a well documented turbulent jet flame (Sandia Flame D). Results are presented and compared with a reference model and measurements.

Keywords: Turbulent combustion; Partial premixing; Reduced chemistry; Flamelets

Nomenclature

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*Corresponding author: giel.ramaekers@gmail.com
Associated Web site: http://www.combustion.tue.nl

1 Introduction
To gain more insight in combustion processes in engineering applications models are developed with the ultimate goal of optimizing fuel-efficiency and minimizing harmful emissions. Many engineering devices, aero-engines for example, operate in a turbulent environment.
regime and fuel and oxidizer are not fully mixed before combustion takes place. The interaction between turbulence and chemistry is still not fully understood and models are developed for the simulation of turbulent, partially-premixed combustion processes.

Turbulent combustion can take place in many different combustion regimes which all have a different interaction between chemistry and turbulence. When turbulence intensity is low turbulent eddies, both macroscopic and microscopic, will not be able to distort the flame which will thus exhibit a quasi-laminar character. With increasing turbulence intensity microscopic eddies will be able to intrude the reaction layer. Macroscopic eddies will be able to deform the flame more severe with increasing turbulence intensity. Borghi [5] defined different regimes and their characteristics. To determine the turbulent combustion regime under aero-engine conditions estimations have to be made for main parameters describing the flow. The mean gas velocity \( U \) in a aero-engine combustor is estimated to be of the order
\[
U = \sqrt{\bar{u} \cdot \bar{u}} = O \left( 10^2 \right) \text{ m/s ,}
\]
and the turbulence intensity \( I \), being the kinetic energy associated with gas velocity fluctuations \( U' \) divided by the kinetic energy associated with mean gas velocity:
\[
I = \frac{U' \cdot U'}{U \cdot U} = 10^{-2}.
\]
This leads to:
\[
U' = O \left( 10^1 \right) \text{ m/s .}
\]
The characteristic length scale of the combustion chamber \( L \) is estimated to be
\[
L = O \left( 10^{-1} \right) \text{ m}.
\]
It is assumed that the integral length scale is equal to the characteristic length scale of the combustion chamber.

For the laminar burning velocity \( s_L \) a small range for the order of magnitude is estimated:
\[
s_L = O \left( 10^{-1} \right) - O \left( 10^0 \right) \text{ m/s}.
\]
For the molecular kinematic viscosity \( \nu \) the order of magnitude well known:
\[
\nu = O \left( 10^{-5} \right) \text{ m}^2/\text{s}.
\]
The assumption is made that diffusion of mass takes place as fast as the diffusion of momentum \( \nu \approx D \). The order of magnitude for the laminar flame thickness \( \delta_L \) can be found by assuming that reaction and diffusion of species are in equilibrium in the reaction layer:
\[
\delta_L \approx \frac{D}{s_L} = O \left( 10^{-5} \right) - O \left( 10^{-4} \right) \text{ m}.
\]
These estimations translate to the turbulent Reynolds number which is the ratio of the inertial and viscous forces:
\[
Re = \frac{U' \cdot L}{\nu} = O \left( 10^5 \right).
\]
The Damköhler number is the ratio of macroscopic turbulent timescale and the chemical timescale. Small Damköhler numbers (\( Da \ll 1 \)) imply a strong deformation of the flame by macroscopic eddies since chemistry is relatively slow. High Damköhler numbers (\( Da \gg 1 \)) imply a very thin flame in which chemical processes take place very fast. For the estimations made the Damköhler number is of the order:
\[
Da = \frac{\bar{t}_c}{t_c} \approx \frac{L \cdot s_L}{U' \cdot \delta_L} = O \left( 10^1 \right) - O \left( 10^3 \right).
\]
The Karlovitz number is the ratio of the chemical timescale and the microscopic turbulent timescale: the Kolmochorov timescale. The Kolmochorov length scale is the lengthscale at which inertial forces are equal to viscous forces; dissipation of turbulent kinetic energy takes place at this scale. Small Karlovitz numbers (\( Ka \ll 1 \)) imply that turbulent eddies can not intrude the flame which will exhibit a laminar character. With increasing Karlovitz numbers (\( 1 < Ka < 100 \)) turbulent eddies will be able to intrude the pre-heat zone of the flame. The Kolmochorov length scale is still larger that the reaction zone of the flame and turbulent eddies can not intrude the reaction zone of the flame. For large Karlovitz numbers (\( Ka \gg 1 \)) no laminar structure can be identified anymore. The Karlovitz number for aero-engine combustor conditions is estimated to be:
\[
Ka = \left( \frac{\tau_c}{\tau_k} \right) = \frac{\delta_L}{L} \left( \frac{U'}{s_L} \right)^{3/2} = O \left( 10^{-1} \right) - O \left( 10^1 \right).
\]
For turbulent premixed combustion these values for \( Re \), \( Da \) and \( Ka \) correspond to the corrugated flamelet regime and the thin reaction zones regime and for turbulent non-premixed combustion these values correspond to the flamelet regime with local extinction. For these regimes the flame thickness is small compared to other length-scales describing the flame. This disables the possibility of describing the chemistry with a perfectly-stirred-reactor (PSR) model. On the other hand the flame thickness can not be assumed to be infinitely thin which disables the possibility of describing the chemistry using a Bray-Moss-Libby (BML) [19], a Eddy-Break-Up (EBU) [19] or a similar model which is based on the assumption that only unburnt and burnt gasses can be present. A turbulent flame can be seen as an ensemble of thin, laminar, locally one-dimensional flames, called flamelets, embedded within the turbulent flow field. For the influence of turbulence an appropriate closure has to be applied. In reality variables like species concentrations and temperature are a function of all other variables. However
the flamelet assumption states that most variables can be assumed to be dependent on a small number of control variables which are relevant for the flamelets which the turbulent flame is thought to be composed of. Turbulent combustion processes have often been modelled assuming that chemistry is much faster than mixing. Mixture fraction, which defines the mass fraction of fuel in the unburnt gas mixture, is one of the main variables describing non-premixed combustion. Flamelets for non-premixed combustion can be generated using a geometry consisting of opposed, axisymmetric fuel and oxidizer jets. As the distance between the jets is decreased and/or the velocity of the jets increased, the flame is strained and increasingly departs from chemical equilibrium until it is eventually extinguished. The use of non-premixed flamelets has become quite common in modelling of turbulent combustion, see [16, 11, 14] for example. Flamelets for premixed combustion can be generated using a geometry with only one inlet in which species are assumed to be perfectly mixed. Chemical reactions will take place as the gas mixture is convected and the mixture composition changes towards chemical equilibrium composition. Partially-premixed combustion is defined as a combustion process in which species are not perfectly mixed before combustion takes place although species are better mixed than in a pure diffusion flame. Partially-premixed combustion can thus be interpreted as a combination of non-premixed and premixed combustion.

Van Oijen [15] showed in simulations of laminar partially-premixed triple flames that a chemical database consisting of premixed flamelets is appropriate for modelling partially-premixed combustion when the length scale affiliated with the gradient in mixture fraction \( Z \) is larger than the flame thickness \( \delta_L \):

\[
\left( \nabla Z \cdot \nabla Z \right)^{-0.5} \gg \delta_L .
\] (1)

For highly turbulent flows mixing occurs very fast and gradients in mixture fraction, \( \nabla Z \), will be small except near inlets when fuel and oxidizer are inserted separately. For such cases it can be assumed that premixed combustion dominates non-premixed combustion. This implies that combustion can be better modelled by using premixed flamelets instead of non-premixed flamelets. For now it is assumed that partially-premixed combustion can be described using an Flamelet Generated Manifold (FGM) consisting of premixed flamelets with mixture fraction covering the entire range between the flammability limits.

The use of premixed flamelets enables the use of a reaction progress variable \( c \) [6] for the description of non-equilibrium chemistry, which defines the local chemical state quantitatively between unburnt and burnt. In case of normalized mass fractions or temperature the reaction progress variable ranges between zero and unity. If mass fractions or temperature are not normalized the reaction progress variable ranges between an initial and final value, which do not have to be equal to zero or unity. For now the common used approach of a normalized reaction progress variable is adopted. It is investigated whether a reaction progress variable, which is directly coupled to chemistry, is a better variable to describe non-equilibrium chemistry than the strain rate in non-premixed flamelets. The strength of FGM reduction technique is that the number independent control variables, which is now chosen to be equal to 2 (\( Z \) and \( c \)), can be increased straightforward for increased accuracy.

When the flamelet based reduction methods like FGM are compared to conventional reduction methods which take only chemical kinetics into account, like the Intrinsic Low Dimensional Manifold (ILDM) reduction technique [8] for example, they prove to be more accurate in regions where chemistry is not dominant (since diffusion is taken into account) and as accurate as conventional reduction methods in regions where chemistry is dominant [15].

The turbulence-chemistry interaction is accounted for by describing variables in a stochastic way instead of a deterministic way: locally a variable is described by a Probability Density Function (PDF) defining the probability of occurrence for several states instead of only one fixed state that can occur. The PDF \( P(x) \) can be thought of as the fraction of time the fluid spends in state \( x \).

For diffusion flames, in which the mixture fraction \( Z \) can be assumed to be the main parameter, the PDF approach is well-known and it has already been implemented in commercial CFD codes like FLUENT [9]. For the introduced reaction progress variable \( c \) an analogous approach is applied to describe the turbulence-chemistry interaction. The only difference is that the transport equation for \( c \) contains a chemical source term while the transport equation for \( Z \) contains no source term.

The objective of this paper is to investigate the FGM/PDF method using premixed flamelets by comparison with existing models and experimental results for a partially-premixed flame, the Sandia flame D. Existing methods that will be considered are the equilibrium chemistry approach and the use of a diffusion flamelet with a fixed strain rate in a flamelet model.

2 Models for turbulent aero-thermochemistry

Three main simulation strategies can be distinguished: Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds Averaged Navier-Stokes Simulation (RANS). In a DNS simulation all turbulent scales down to the Kolmohorov scale are resolved which implies that computational costs are very high. A comparison of the integral length scale with the Kolmohorov length scale and the integral time scale with the Kol-
mochorov time scale shows that, for non-reacting flows, computational requirements $CR_{NR}$ scale with:

$$CR_{NR} \sim \frac{Re^{2.25}}{Re^{0.5}} \cdot \frac{Da}{time} = Re^{2.75}.$$  

For turbulent reacting flows the reaction layer has to be captured properly and computational requirements $CR_R$ will not only be determined by the Reynolds number but by the Damköhler number as well [19]:

$$CR_R \sim \frac{(Re Da)^{1.5}}{space} \cdot \frac{Da}{time} = [Re^3 Da^5]^{0.5}.$$  

The most severe requirement ($CR_{NR}$ or $CR_R$) determines the total required computational facilities for simulations of turbulent reactive flows. The Reynolds number and/or Damköhler number for which DNS simulations can be run are thereby limited by the available computational facilities.

The LES approach reduces the requirements on computers by only simulating the largest turbulent eddies and modelling small eddies. This approach is justified by the fact that the large eddies are far more important for the turbulent diffusion of species, momentum and heat than small eddies [17]. Since the flame can still be thinner than the numerical cell size, for turbulent combustion models usually can not be as simplified as the subgrid turbulence model.

In RANS simulations turbulent eddies are not resolved. In both RANS and LES simulations models have to be used to account for the eddies that are not resolved. This is the so called “closure-problem” for the unknown correlations that occur in the PDE’s describing turbulent reacting flows. For the modelling of turbulent combustion under aero-engine conditions the RANS approach has been chosen because the complex geometry of an aero-engine combustion chamber would make LES and DNS simulations too time-consuming.

To model turbulence, the realizable $k, \epsilon$-model [14, 9] which solves equations for the turbulent kinetic energy $k$ and the turbulent kinetic energy dissipation rate $\epsilon$ is used. Dimensional analysis leads to an expression for an additive turbulent viscosity which is a function of the geometry; it is not a property of the working fluid. The realizable $k, \epsilon$-model is more suitable for axisymmetric jet flames than the standard $k, \epsilon$-model [9].

Chemistry is represented by the GRI3mech 3.0 mechanism [23] which contains 325 elementary reactions between 53 species with hydrocarbons up to propane; it is important to include higher hydrocarbons than present in the fuel to be able to describe hydrocarbon recombination in rich regions. This is why a relative simple reaction mechanism like the Smooke reaction mechanism [24] will not suffice in methane flames containing rich regions.

2.1 Partially-premixed combustion parameters

To describe partially-premixed combustion two control parameters describing non-premixed (mixture fraction $Z$) and premixed combustion (reaction progress variable $c$) are important, as explained in section 1.

The mixture fraction is a conserved scalar which describes the conservation of elements. According to Bilger [4] the mixture fraction is defined as [3]:

$$Z = \begin{cases} 
0.5 & \frac{Y_H - Y_{H,2}}{M_H} + 2.0 \frac{Y_C - Y_{C,2}}{M_C} \\
0.5 & \frac{Y_{H,1}-Y_{H,2}}{M_H} + 2.0 \frac{Y_{C,1}-Y_{C,2}}{M_C} 
\end{cases},$$  

in which the subscript $H$ denotes hydrogen, the subscript $C$ denotes carbon, the subscript 1 denotes the fuel inlet and the subscript 2 denotes the oxidizer inlet. $M_H$ represents the element mass of hydrogen and $M_C$ represents the element mass of carbon. When it is assumed that diffusion coefficients are equal for all species, the transport equation for the mixture fraction is described by [19]:

$$\nabla \cdot \left[ \tilde{\rho} \tilde{u} \tilde{Z} \right] - \nabla \cdot \left[ \tilde{\rho} \left( D + D_T \right) \nabla \tilde{Z} \right] = 0,$$  

which is derived by applying the single-perturbation theory and subsequently Reynolds averaging the equation describing the transport of $Z$ in laminar flows. The transport by convection and diffusion has been marked in this equation for clarity; they will not be marked in following equations. Mixture fraction has no source term since mixture fraction is a conserved scalar. Molecular diffusion is modelled by Fick’s diffusion law with diffusion coefficient $D$ and turbulent diffusion is modelled in a similar way using the Boussinesq approximation which introduces a turbulent diffusion coefficient $D_T$. The use of Fick’s diffusion law and an analogous approach for the influence of turbulence implies that preferential diffusion and counter-gradient diffusion can not occur.

A random Favre averaged, or mass-averaged, variable $\varphi$ is defined as:

$$\tilde{\varphi} = \frac{\varphi \tilde{\rho}}{\tilde{\rho}},$$  

in which $\tilde{\rho}$ is the Reynolds averaged density. Favre averaged variables are introduced to prevent terms containing density fluctuations for which closure assumptions have to be made.

For the reaction progress variable $c$ an indicator has to be chosen which discriminates between unburnt, burnt and intermediate stages. For $c$ the requirement must be posed that it is monotonous from the initial state to chemical equilibrium in order to facilitate an unambiguous determination of dependent variables as a function of $c$. Straightforward choices for $c$ could be mass fractions of reactants or products, a linear combination of species
mass fractions or gas temperature. The choice made for \( c \) in this study will be presented in section 2.4. The transport equation for \( c \) is derived analogous to the transport equation for \( Z \); the only difference is the presence of a chemical source term on the right hand side. It is described by

\[
\vec{\nabla} \cdot \left[ \frac{\rho \vec{u}}{\rho} \right] = \frac{\rho \vec{u}}{\rho} + \vec{D} .
\]

Both laminar diffusion of \( c \) and diffusion of \( c \) due to turbulent fluctuations is modelled similar to diffusion of the mixture fraction.

In all transport equations molecular diffusion is not assumed to be much smaller than the redistributive flux due to turbulent fluctuations since in very hot regions with low turbulence intensities molecular diffusion can play a significant role in diffusion of species, momentum and heat. For both \( Z \) and \( c \) molecular diffusion coefficients are related to molecular viscosity using laminar Schmidt numbers \( Sc \) and turbulent diffusion coefficients are related to turbulent viscosity using turbulent Schmidt numbers \( Sc_T \) according to:

\[
D = \frac{\nu}{Sc} ; \quad D_T = \frac{\nu_T}{Sc_T} .
\]

Turbulent Schmidt numbers can be expected to take values closer to unity than laminar Schmidt numbers since transport by turbulent fluctuations can be expected to be more for momentum and species than transport by molecular processes. For the mixture fraction in literature [9, 13] laminar and turbulent Schmidt numbers are found equal to 0.7 and 0.85 respectively; these Schmidt numbers will also be used in this study. For the reaction progress variable the same Schmidt numbers are taken.

2.2 PDF closure method

As explained in section 1 turbulence influences the combustion chemistry by distorting the flame. A stochastic description of variables is appropriate for the regimes as mentioned in section 1. All variables are described as an ensemble of different realizations each with a certain probability of occurrence. Using the flamelet approach it is assumed that all variables are only a function of mixture fraction \( Z \) and reaction progress variable \( c \): \( \varphi = \varphi(Z, c) \). Variables are from here on described stochastically by mass-weighted PDF’s, \( \tilde{P}(Z, c) \) and a Favre averaged variable is calculated according to:

\[
\tilde{\varphi} = \int_{0}^{1} \int_{0}^{1} \varphi(Z, c) \tilde{P}(Z, c) dZ dc .
\]

For the Reynolds averaged density and Reynolds averaged source term for \( c \) a conversion has to be introduced to be able to use the same mass-weighted PDF’s for Favre averaged variables. The Reynolds averaged density \( \overline{\rho} \) is given by:

\[
\overline{\rho} = \left[ \frac{1}{\rho} \right]^{-1} = \left[ \int \int \tilde{P}(Z, c) dZ dc \right]^{-1} .
\]

The Reynolds averaged source term \( \overline{\omega} \) can be written as:

\[
\overline{\omega} = \rho \left[ \frac{\tilde{\omega}}{\rho} \right] = \frac{\tilde{P}(Z, c)}{\rho} .
\]

The shape of the joint mass-averaged PDF, \( \tilde{P}(Z, c) \), is not known but can be computed by using expensive methods like Monte-Carlo simulations [21] or the use of transported PDF’s [5, 14, 21]. A more simple approach is a PDF approach. The assumption that \( Z \) and \( c \) are statistically independent is used allowing the joint PDF \( \tilde{P}(Z, c) \) to be written as the product of its two marginal PDF’s:

\[
\tilde{P}(Z, c) = \tilde{P}(Z) \tilde{P}(c)
\]

Subsequently known shapes that can be described by a small number of parameters are presumed for the two marginal PDF’s. In this study it is assumed that the shape of each of the two marginal PDF’s can be described by a mean and a variance implying that all variables become a function of mean mixture fraction \( \tilde{Z} \), mean reaction progress variable \( \tilde{c} \), variance of mixture fraction \( \xi \) and variance of progress variable \( \phi \). Since \( Z \) and \( c \) can be decomposed to a mass-averaged mean, \( \tilde{Z} \) respectively \( \tilde{c} \), and a fluctuation, \( Z' \) respectively \( c' \), for \( \xi \) and \( \phi \) can be written:

\[
\xi = \left( Z - \tilde{Z} \right)^2 = Z' \xi \quad \text{and} \quad \phi = \left( c - \tilde{c} \right)^2 = c' \phi .
\]

A transport equation for a variance can be derived by multiplying a standard transport equation for a variable with the fluctuation of that variable and subsequently apply Reynolds averaging. The transport equation for the variance of the mixture fraction \( \xi \) reads:

\[
\vec{\nabla} \cdot \left[ \frac{\nu \tilde{\xi}}{\rho} \right] = 2C_1 \overline{\rho} D_T \left( \vec{\nabla} \tilde{Z} \right)^2 - 2C_2 \overline{\rho} \chi_\xi ,
\]

in which \( C_1 \) and \( C_2 \) are modelling constants. In this derivation the assumption that \( \xi \) and its destruction, \( \chi_\xi \), scales linear to the turbulent kinetic energy \( k \) and its destruction rate \( \epsilon \) according to:

\[
\chi_\xi = \frac{\epsilon}{k} \xi
\]

In this study \( C_1 \) and \( C_2 \) have been given the values used in FLUENT [9]: \( C_1 = 1.215 \) and \( C_2 = 1 \). This is done for reasons that will be explained later.
The transport equation for the reaction progress variable variance \( \phi \) is described by:

\[
\nabla \cdot \left[ \overline{\rho \dot{\phi}} - \overline{p (D + D_T) \nabla \phi} \right] = 2C_3 \overline{p D_T} + \overline{2C_4\overline{\omega} - 2C_5 \overline{\phi} \left( \frac{s}{k} \right)} \phi
\]

in which \( C_3, C_4 \) and \( C_5 \) are modelling constants. For the destruction of \( \phi \) the same coupling to the \( k, e \) turbulence model as for \( \xi \), as stated in equation 9, has been applied. Equation 10 contains an additional source term \( \overline{c \omega} \) when compared to equation 8 for the variance of the mixture fraction. This additional source term occurs due to the source term in equation 4 and is defined as:

\[
\overline{c \omega} = \overline{c \omega} - \overline{\omega c}.
\]

\( \overline{\omega} \) is defined according to equation 7 and \( \overline{c \omega} \) is, analogous to equation 7, defined as:

\[
\overline{c \omega} = \overline{\rho \int \frac{c \omega(Z, c)}{\rho(Z, c)} \frac{\overline{\rho p}}{\overline{\rho p}} \overline{\rho p} \overline{\rho p} dZdc}.
\]

For the variance of the mixture fraction the laminar and turbulent Schmidt numbers are assumed to be equal to 0.7 and 0.85, respectively [13]. For the reaction progress variable variance the same Schmidt numbers are assumed, similar to the assumption made for the reaction progress variable. Modelling constants \( C_3 \) to \( C_5 \) are kept equal to unity in this study.

The laminar viscosity, which is used to calculate molecular diffusion coefficient \( D \) according to equation 5, is determined using the Sutherland law for air. Since the laminar viscosity can be assumed to be quasi-linear dependent on temperature it can be determined using the Favre-averaged temperature \( \overline{T} \). Hereby a complex PDF integration like for the averaged source term (equation 7) is circumvented. The expression for the laminar viscosity reads:

\[
\nu = \frac{\mu_0}{\overline{\rho}} \left( \frac{\overline{T}}{T_0} \right)^{1.5} \left[ \frac{T_0 + A}{\overline{T} + A} \right]
\]

in which the modelling constants \( \mu_0, T_0 \) and \( A \) have been taken equal to those for air [9]:

\[
\mu_0 = 1.7894 \cdot 10^{-5} ; \quad T_0 = 273.11 ; \quad A = 110.56
\]

The choice to use the same modelling constants as for air is funded on the assumption that laminar viscosity will only play a role in hot regions with a low turbulence intensity. This typically is the burnt-out region in which burnt gases are further mixed with excess air implying that gas mixture composition will resemble the composition of air relatively well.

2.3 Assumed PDF shape

Since mixture fraction and progress variable are bounded variables a PDF with a bounded domain is preferred over PDF’s with a non-bounded domain. The \( \beta \)-distribution is a bounded PDF for \( x \in [0, 1] \) and according to FLUENT [9] it most closely represents experimentally observed PDF’s. The \( \beta \)-distribution is described by:

\[
\dot{P}(x; p, q) = \frac{\Gamma(p + q)}{\Gamma(p) \Gamma(q)} x^{p-1} (1 - x)^{q-1}
\]

in which the gamma-function \( \Gamma \) is defined as [1]:

\[
\Gamma(p) = \begin{cases} \int_0^\infty t^{p-1} e^{-t} dt & \text{if } p \text{ is continuous} \\ (p - 1)! & \text{if } p \text{ is discrete} \end{cases}
\]

The two parameters \( p \) and \( q \) in the \( \beta \)-distribution (stated in equation 12) are related to the mean, \( \mu \), and variance, \( \sigma^2 \), according to:

\[
p = \mu \left( \frac{1 - \mu}{\sigma^2} - 1 \right) > 0
\]

\[
q = (1 - \mu) \left( \frac{1 - \mu}{\sigma^2} - 1 \right) > 0
\]

When the PDF for \( Z \) is considered \( \mu \) and \( \sigma^2 \) in equation 14 and 15 are:

\[
\mu = \bar{Z} ; \quad \sigma^2 = \xi = \frac{\overline{z\overline{\omega}}} \in [0, \bar{Z} \left(1 - \bar{Z}\right)]
\]

and for the PDF for \( c \):

\[
\mu = \bar{c} ; \quad \sigma^2 = \phi = \frac{\overline{c\overline{\omega}}} \in [0, \bar{c} \left(1 - \bar{c}\right)]
\]

It can be concluded that the PDF for mixture fraction is a function of mean mixture fraction, \( \bar{Z} \), and mixture fraction variance:

\[
\dot{P}(Z) = \dot{P}\left(Z; \bar{Z}, \overline{z\overline{\omega}}\right) = \dot{P}\left(Z; \bar{Z}, \xi\right).
\]

The PDF for the reaction progress can be written analogous:

\[
\dot{P}(c) = \dot{P}\left(c; \bar{c}, \overline{c\overline{\omega}}\right) = \dot{P}(c; \bar{c}, \phi).
\]

2.4 Determination of the laminar source term \( \omega \)

To be able to use the FGM/PDF method one must be able to compute the Reynolds-averaged source for the reaction progress variable, \( \overline{\omega c} \), which depends on the laminar variable \( \omega_c (Z, c) \) according to equation 7. According to the flamelet assumption, as explained in section 1, laminar variables can be retrieved from laminar flamelets when \( Z \) and \( c \) are known. A schematic comparison between the use of non-premixed and premixed flamelets is given in figure 1 in which \( c_{\text{max}} \) is the maximum value for \( c \) that can be achieved for non-normalized variables at stoichiometric combustion; if normalized variables are concerned \( c \) ranges between zero and unity. It can be seen that diffusion flamelets contain chemical information beyond flammability limits which is not included in a database consisting of premixed flamelets. On the other
hand non-equilibrium chemistry is expected to be better represented using premixed flamelets since then the entire range for the reaction progress variable \( c \) is included; diffusion flamelets reduce to a pure mixing problem beyond the maximum strain rate.

For the reaction progress variable \( c \) still an appropriate choice has to be made and several options are available: a major reactant mass fraction or major product mass fraction would be a straightforward option. A more refined option would be a linear combination of multiple species mass fractions to ensure a monotonous reaction progress variable in both lean and rich regions; a possible combination could include CO\(_2\), H\(_2\)O, CO and H\(_2\) [2] of which the first two are typical products for lean combustion and the latter two are typical products for rich combustion.

The reaction progress variable ranges from zero to unity; species mass fractions or a linear combination of multiple species mass fractions will typically not be in the same range! Scaling a species mass fraction or a linear combination of multiple species mass fractions between zero and unity will introduce additional terms in equation 4 [12, 6] (due to the dependence of \( c_{\text{max}} \) on \( Z \)): scaling of \( c \) is assumed to reduce the dependence of \( c \) on \( Z \) [12].

In this study the mass fraction of CO\(_2\) is chosen as a reaction progress variable: \( c = Y_{\text{CO}_2} \). It satisfies the requirement to be monotonous increasing between the flammability limits given by Cashdollar et al [7].

\[ X_{\text{CH}_4} \in [0.05, 0.15], \text{ when the GRI mech 3.0 reaction mechanism is used. The maximum value for } c \text{ is a function of } Z \text{ but in this study it is assumed that } c \text{ and } Z \text{ can nevertheless be considered statistically independent and a non-scaled reaction progress variable is used to avoid additional terms in equation 4.} \]

The laminar chemical database consisting of premixed flamelets is generated using the flamelet code CHEM1D [10] which solves all PDE’s describing laminar combustion [19]. Heat transfer by means of radiation is not included. There can be no interaction between flamelets. A flamelet is represented by a large number of discrete points and an adaptive grid makes sure that the reaction layer is captured well. It must be noted that boundary conditions for dependent variables must correspond to boundary conditions encountered in simulations in which the laminar chemical database will be used.

### 2.5 Numerical procedures

To decrease computational costs the use of a structured pre-integrated chemical database and an interpolation routine in the CFD code is preferred over an integration routine inside the CFD code [9].

In order to generate a pre-integrated chemical database two steps have to be taken: first a laminar flamelet database has to be generated and subsequently the laminar flamelet database has to be integrated over multiple, different PDF’s for \( Z \) and \( c \).

As stated in section 2.2 in the laminar flamelet database all variables are defined as a function of mixture fraction \( Z \) and reaction progress variable \( c \): \( \varphi = \varphi(Z, c) \). As an example the laminar source term for CO\(_2\), which is required to compute the Reynolds averaged source term for \( c, \bar{\omega}_c \), is shown in figure 2.

The PDF integration routine integrates the laminar flamelet database with a shape for the PDF’s of \( Z \) and \( c \) defined by \( \bar{Z}, \xi, \bar{c} \) and \( \phi \). All Favre-averaged variables are defined by a combination of mean mixture fraction \( \bar{Z} \), mixture fraction variance \( \xi \), mean reaction progress variable \( \bar{c} \) and reaction progress variable variance \( \phi \): \( \bar{\varphi} = \bar{\varphi}(\bar{Z}, \xi, \bar{c}, \phi) \). This procedure is performed for multiple combinations of \( \bar{Z}, \xi, \bar{c} \) and \( \phi \) and averaged \( \bar{\varphi} \) are stored in a structured database so that they can be retrieved as a function of \( Z, \xi, \bar{c} \) and \( \phi \). A fast look-up procedure to retrieve chemical data during a CFD computations is possible since the location of the requested data in the integrated database can be determined directly due to the known structure of the database. Figure 3 shows the dependence of the Reynolds averaged source term for \( c, \bar{\omega}_c \), on the normalized mixture fraction variance and normalized reaction progress variable variance at \( \bar{Z} = 1.03Z_{\text{st}} \) and \( \bar{c} = 0.5c_{\text{max}}(Z_{\text{st}}) \). These values for \( \bar{Z} \) and \( \bar{c} \) correspond to the region in the laminar chemical database where the laminar source term for \( c, \bar{\omega}_c \) reaches its maximum.

---

Figure 1: Schematic comparison between non-premixed flamelets (blue lines) and premixed flamelets (black lines). The red line, also indicated by \( \chi^0 \), represents chemical equilibrium corresponding to a non-premixed flamelet with a strain rate equal to zero. The blue line indicated by \( \chi_{\text{max}} \) represents the non-premixed flamelet at its extinction limit. LFL denotes the lower flammability limit and UFL denotes the upper flammability limit.
value as can be seen from figure 2.

To compute the incomplete $\beta$-function as defined by equation 12, Numerical Recipes [20] recommends a polynomial for the $\Gamma$-function described in equation 13. For the integral of the $\beta$-distribution $P(x; p, q)$, as described in equation 12, a continued fraction approach is recommended [20]. For optimal numerical efficiency the PDF integration routine contains three innovative routines:

1. Gridpoints are clustered in area’s where the PDF has relatively large values using an adaptive grid. During integration the domains for $Z \in [0, 1]$ and $(c/c_{\text{max}}) \in [0, 1]$ are divided in multiple subdomains; it is made sure that the integrated probability of each subdomain is equal by using a Newton iteration containing the PDF and the cumulative probability density function (CDF) to find the bounding coordinates of each subdomain.

2. Integration points are placed in the middle of the bounding coordinates of each subdomain which have been determined by the adaptive gridding routine. This can cause the real mean and variance to differ slightly from the imposed mean and variance. To reconstruct the imposed mean and variance the real mean and variance, which can be computed from the integration points and the PDF, are modified by scaling the PDF height and introducing two Dirac functions at the extremes of the domain (for the mixture fraction $Z = 0$ and $Z = 1$ and for the reaction progress variable $c = 0$ and $c = c_{\text{max}}$).

3. The PDF-averaged variables are calculated on an initial grid and subsequently on a more refined grid with twice the number of gridpoints in both directions ($Z$ and $c$). The PDF-averaged variables computed on the finer grid are compared to the values on the previous, more coarse grid. This process is repeated until a convergence criterion is reached which is based on the Reynolds averaged density $\rho$ and the Reynolds averaged source term for the progress variable $\overline{\dot{c}}$ and is set to $10^{-3}$. The maximum number of subdomains in both directions was set to 160.

3 Results

The FGM/PDF model will be compared to an established model for turbulent combustion to prove its concept. The comparison will be made for a well-known test case to be able to compare numerical results for both models with experimental data in order to point out advantages and disadvantages of the FGM/PDF concept.

3.1 Description test case

The Sandia Flame D was chosen as a test case. It is a piloted jet diffusion flame. This flame is chosen from a series of flames, ranging from laminar (Flame A) to highly turbulent (Flame F). Flame D (Re=22,400 based on fuel inlet diameter) is a turbulent flame for which measurement data of both the flow (velocities and turbulence) [22] and species [3] is available. Since the turbulence-chemistry interaction is only moderate
there is no clear advantage for the FGM/PDF model beforehand. Because the fuel is premixed with air recombination of hydrocarbons and the production of soot are reduced. This allows the use of the GRImech 3.0 mechanism \[23\] which includes hydrocarbons up to propane.

The fuel inlet is a cylindrical tube with a diameter of \(d = 7.2\) mm and the fuel consists of \(X_{\text{CH}_4} = 0.25\) and \(X_{\text{air}} = 0.75\). It is surrounded by a pilot inlet tube, having a diameter of \(18.2\) mm. In the pilot mixture fraction \(Z\) equals \(0.77\) \(Z_{\text{st}}\) and the gas mixture composition equals the chemical equilibrium composition for this value of \(Z\). The burner is placed in a wind tunnel blowing only air. The computational geometry for the Sandia Flame D is shown in figure 4. A structured numerical grid consisting of 40,000 cells with refinements on the inlets and along the axis of symmetry, the \(y\)-axis, is used for computations on the geometry shown in figure 4. The radial coordinate is indicated by \(r\). The smallest cell has a surface of \(0.26\) mm\(^2\), the largest cell has a surface of \(1.7 \cdot 10^3\) mm\(^2\).

In the inlets at \(y = 0\) (air, pilot and fuel) the axial velocity, turbulent kinetic energy and turbulent kinetic energy dissipation rate inlet profiles are prescribed by measured profiles [3]. For mixture fraction and reaction progress variable values see table 1. The value for \(c\) in the pilot inlet corresponds to the chemical equilibrium value of \(c\) for the value of \(Z\) in the pilot inlet which implies that all values in the pilot inlet are equal to chemical equilibrium values. For the tube walls a no-slip boundary condition is prescribed. For the outlet a constant pressure, dictated by the Sandia Flame D description [3], which is equal to the inlet pressure is prescribed: \(p = 1.0062 \cdot 10^5\) Pa. Under the assumption that at \(r = 300\) mm radial velocities approximately equal zero, a zero-shear wall has been used as a far-field boundary condition.

<table>
<thead>
<tr>
<th>Inlet</th>
<th>(Z)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel inlet</td>
<td>1.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Pilot inlet</td>
<td>0.27</td>
<td>0.1156</td>
</tr>
<tr>
<td>Air inlet</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Table 1: Mixture fraction \((Z)\) and reaction progress variable \((c)\) inlet conditions.

### 3.2 Accuracy integrated database

The laminar chemical database generated using the FGM reduction method as described in section 2.4 is created for the Sandia Flame D fuel inlet boundary conditions [3]: \(T = 294\) K and \(p = 1.0062 \cdot 10^5\) Pa. For the domain between the flammability limits the values \(X_{\text{CH}_4} \in [0.05, 0.15]\) have been used which correspond to values for the mixture fraction equal to \(Z \in [0.18, 0.56]\). The laminar chemical database contained 101 flamelets each discretized in 80 points using an adaptive grid to capture the reaction layer. The adaptive grid made sure that the increase of \(\text{CO}_2\) between two subsequent points was equal over the entire domain.

During the integration procedure values for \(Z\) outside the flammability limits variables are interpolated. For values for \(Z\) below the lower flammability limit variables are interpolated between the oxidizer stream and the leanest flamelet. When values for \(Z\) are beyond the upper flammability limit variables are interpolated between the richest flamelet and the fuel stream. For the integrated table 26 uniformly distributed mixture fraction values have been taken to properly capture the expected maximum value for \(c\) and \(T\), which lies a few percent on the rich side of \(Z_{\text{st}} = 0.351\) in the laminar chemical database. The reaction progress variable \(c\) is represented by 20 linearly distributed values. For both the mixture fraction variance \(\xi\) and reaction progress variable variance \(\phi\) 10 values are taken. Values for variances are clustered more dense for small values since integrated variables show a strong dependence on variances for small values of variances. Clustering of values for
and as it is retrieved from the integrated table using linear interpolation: it shows that the temperature is captured well using linear interpolation in combination with the chosen distribution for \( Z \) and \( c \).

\[ T \text{ [K]} \]

![Figure 5: Temperature at chemical equilibrium as a function of mixture fraction for the laminar chemical database (circles) and the PDF-integrated database (solid line).](image)

In figure 5 the temperature at chemical equilibrium as a function of mixture fraction is shown for both the FGM and as it is retrieved from the integrated table using linear interpolation: it shows that the temperature is captured well using linear interpolation in combination with the chosen distribution for \( Z \) values. When the interpolation error \( \epsilon \) is defined as

\[
\epsilon = \left| \frac{z_T - z_L}{z_T} \right|
\]

in which subscript \( L \) denotes data from the laminar database and subscript \( T \) denotes data from the integrated database, the maximum error is reached at \( Z = 0.98 Z_{\text{ex}} \) and is less than 1%.

In figure 6 the temperature at stoichiometric mixture fraction as a function of the reaction progress variable is shown for both the FGM and as it is interpolated from the integrated table. Since the profile does not have any sharp peaks, it is reproduced very well using linear interpolation between 20 values for the reaction progress variable \( c \). There is a very small region \( (c/c_{\text{max}} \in [0, 0.05]) \) where errors up to 10% occur. Outside this region errors are always less than 0.5%. The same definition for the interpolation error \( \epsilon \) is used.

3.3 Comparison of results for the FGM/PDF method

To show the importance of the inclusion of both reaction progress variable and the turbulence-chemistry interaction for the reaction progress variable three versions FGM/PDF models are compared:

1. **Full FGM/PDF model**: equations for \( Z \), \( c \), \( \xi \) and \( \phi \) are solved. This model contains non-equilibrium chemistry and the interaction between turbulence and chemistry for both \( Z \) and \( c \).

2. **Reduced FGM/PDF model**: only equations for \( Z \), \( c \) and \( \xi \) are solved. The equation for the variance for the reaction progress variable \( \phi \), equation 10, is excluded from the set of equations and \( \phi \) is taken equal to zero. This exclusion implies that the PDF for \( c \) is always represented by a Dirac \( \delta \)-function at \( \hat{c} \).

3. **Chemical equilibrium FGM/PDF model**: both equations for \( c \) and \( \phi \) are excluded from the set of equations. This implies that convection and diffusion for \( c \) are not accounted for. Chemistry is assumed to be infinitely fast \( (c = c_{\text{max}}) \) and mixing is rate-limiting.

As reference model a diffusion flamelet from a counterflow flame with a strain rate of 100 s\(^{-1}\) has been used [11]. This moderate strain rate has been chosen because the diffusion flamelet should exhibit only little local extinction corresponding to experimental data. This laminar chemical database has been integrated with a \( \beta \)-PDF using PRE-PDF included in FLUENT.

The results of the model consist of variables of the flow and the combustion chemistry. First two main properties of the flow, the axial velocity and the turbulent kinetic energy \( k \), are discussed because they determine mixing processes. Numerical results for all FGM/PDF models and the diffusion flamelet model are compared to experimental data of Schneider et al [22].

In figure 7 the axial velocity \( U_{\text{ax}} \) on the symmetry axis is presented for the all FGM/PDF models and the diffusion flamelet model. All models predict approximately the same values for the velocity magnitude in the entire domain; for \( 35 < y/d < 75 \) predictions from the FGM/PDF model are slightly closer to measurements. In figure 8 predictions of the turbulent kinetic energy along the symmetry axis show that the maximum value predicted by all versions of the FGM/PDF model is approximately 10% higher than predicted by the diffusion flamelet model. The shapes of both curves are similar. Both models predictions only correspond to experimental data in the downstream part (\( y/d > 40 \)): the broad plateau for \( 20 < y/d < 40 \) is not predicted by
Now that the main properties of the flow are described a closer look is taken at the combustion process. Predicted values for mixture fraction and combustion scalars are compared to experimental data of Barlow et al [3].

Thus figure 9 presents the mean mixture fraction $\bar{Z}$ on the symmetry axis for all models together with experimental measurements. It shows that all FGM/PDF models predict similar values. For $20 < y/d < 60$ the diffusion flamelet model predicts values for $\bar{Z}$ that are slightly higher than the FGM/PDF models. This is caused by predicted values for $k$ which are lower for the diffusion flamelet model than for the FGM/PDF models for $20 < y/d < 40$ as has been shown in figure 8. There is no clear advantage of the FGM/PDF models over the diffusion flamelet model or vice versa for predictions of $\bar{Z}$.

In figure 10 can be seen that the shape of the curve for the variance of the mixture fraction ($\xi$) is similar for all FGM/PDF models and the diffusion flamelet model although the position at which the maximum value for $\xi$ is reached is better predicted by the diffusion flamelet model. All FGM/PDF models overpredict the maximum value for $\xi$; the diffusion flamelet model underpredicts the maximum value for $\xi$. Predictions made by the diffusion flamelet model correspond better to measurements than predictions made by any FGM/PDF model. For all FGM/PDF models modelling constants in equation 8 have been taken equal to constants used by FLUENT [9] to facilitate a fair comparison with the diffusion flamelet model.
Figure 11 presents the mean reaction progress variable $\tilde{c}$ on the symmetry axis for all models together with experimental measurements. In the upstream region $y/d < 60$ ($d$ denotes the fuel inlet diameter) there is a clear discrepancy between all FGM/PDF models on one hand and the diffusion flamelet model and experimental data on the other hand. In this region the flame is not in equilibrium. Predictions made by the diffusion flamelet model correspond better to measurements than predictions made by any FGM/PDF models. In the downstream region $y/d > 60$ the reduced- and chemical equilibrium FGM/PDF model predictions converge towards the diffusion flamelet predictions.

For $30 < y/d < 40$ a clear distinction is visible between the chemical equilibrium FGM/PDF model on one hand and the reduced- and full FGM/PDF model on the other hand: the chemical equilibrium underpredicts values for $\tilde{c}$. This is explained by the fact that in the chemical equilibrium model convection and diffusion of $\tilde{c}$ is not included. Since there is a large radial gradient in $\tilde{c}$ at the symmetry axis for $20 < y/d < 40$, as can be seen in figure 12, convection and diffusion will play an important role in the transport of $\tilde{c}$ towards the symmetry axis. These transport phenomena are included in the reduced- and full FGM/PDF models and therefore these models are assumed to be more accurate. For $60 < y/d < 80$ the predictions for $\tilde{c}$ made by the full FGM/PDF model correspond better to experimental data than all other models. This can be explained by equation 1: in regions with small gradients in $Z$, like the downstream part of the computational domain, chemistry can be represented better using premixed flamelets than using non-premixed flamelets. In contrary, the upstream part $y/d < 60$, where gradients in $Z$ are large, combustion can be better represented by using non-premixed flamelets. This explains why the diffusion flamelet model yields better results in the upstream part of the computational domain.

In figure 14 temperature predictions made by all FGM/PDF models are compared to predictions made by the diffusion flamelet model and measurements. In the upstream part $y/d < 40$ predictions made by the reduced- and chemical equilibrium FGM/PDF models correspond almost exactly to predictions made by the full FGM/PDF model. In the downstream part the predictions made by the reduced- and chemical equilibrium FGM/PDF resemble the predictions of the diffusion flamelet model better than the predictions made by the full FGM/PDF model. In the upstream part $y/d < 55$ the diffusion flamelet approach corresponds better to measurements; in the downstream part ($y/d > 55$) the full FGM/PDF model using premixed flamelets predicts values closer to measurements.

The small wiggle at $y/d \approx 45$ in the temperature profile predicted by the full FGM/PDF model is most probably caused by the wiggle in the predicted profile for $\phi$ as

\[ \phi = \frac{\Delta c}{c} \]

The reaction progress variable variance $\phi$ predicted by the full FGM/PDF model is shown in figure 13 together with the mean reaction progress variable $c$. They are plotted together to point out that the location of the wiggle in $\phi$ ($y/d \approx 45$) corresponds to the location of the maximum value for $\tilde{c}$. According to equation 10 the production of $\phi$ scales with the square of the spatial gradient of $\tilde{c}$; when a local maximum (or minimum) of $\tilde{c}$ is reached spatial gradients of $\tilde{c}$ equal zero and there will be no production of $\phi$. If the influence of convection and diffusion is assumed to be constant in the region close to the peak in $\tilde{c}$ the value for $\phi$ will decrease since destruction is a non-zero value. The predicted trend is similar to experimental data but the full FGM/PDF model overpredicts $\phi$ for $30 < y/d < 55$ and underpredicts $\phi$ for $55 < y/d < 80$.

**Figure 11:** Axial profile ($r = 0$) of the mean reaction progress variable $\tilde{c}$ for the full FGM/PDF model (solid line), the reduced FGM/PDF model (dotted line), the chemical equilibrium FGM/PDF model (dash-dotted line) and the diffusion flamelet model (dashed line) together with measurements (circles).

**Figure 12:** Radial profile of the mean reaction progress variable $\tilde{c}$ for the full FGM/PDF model at $y/d = 20$ (solid line), $y/d = 30$ (dashed line) and $y/d = 40$ (dotted line). Convection and diffusion of $c$ is included in the full FGM/PDF model.
shown in figure 13. This conviction is confirmed by the fact that predictions made by the reduced- and chemical equilibrium FGM/PDF model, in which no equation for $\phi$ is solved and $\phi$ is set to zero, do not exhibit this wiggle.

In figure 15 the methane mass fraction, $Y_{CH_4}$, predictions made by the full FGM/PDF model and the diffusion flamelet model together with measurements are shown. The diffusion flamelet model predictions correspond better to measurements than predictions made by the full FGM/PDF model.

Figure 16 shows the oxygen mass fraction, $Y_{O_2}$, predictions made by the full FGM/PDF model and the diffusion flamelet model together with measurements. Similar to figure 11 the diffusion flamelet model yields better predictions in the upstream region $y/d < 60$ and the full FGM/PDF model gives better predictions in the downstream region $60 < y/d < 80$.

Figure 17 shows radial profiles for the mean mixture fraction $\bar{Z}$ and the mixture fraction variance $\phi$ predicted by the full FGM/PDF model and the diffusion flamelet model together with measurements. Radial profiles have been taken at three heights from the inlets: $y/d = 15$, $y/d = 45$ and $y/d = 75$. Similar to predictions at the symmetry axis shown in figure 9 there is no model of which its predictions correspond better to measurements than other models. For predictions of the mixture fraction variance the diffusion flamelet model corresponds slightly better to measurements than predictions made by the full FGM/PDF model.

In figure 18 radial profiles for the mean reaction progress variable $\bar{\epsilon}$ and temperature $T$ are shown at the same distances from the inlets as figure 17. The radial profiles for $\bar{\epsilon}$ at $y/d = 15$ and $y/d = 45$ show that the full FGM/PDF overpredicts values for $\bar{\epsilon}$. This is in correspondence to the axial profile for $\bar{\epsilon}$ predicted by the full FGM/PDF model as shown in figure 11.
Figure 17: Mean mixture fraction $\bar{Z}$ and mixture fraction variance $\xi$ as a function of radius at three heights above the inlet plane: $y/d = 15$, $y/d = 45$ and $y/d = 75$. The full FGM/PDF model (solid line) and the diffusion flamelet (dashed line) are shown together with measurements (circles).

Figure 18: Mean reaction progress variable $\bar{c}$ and temperature $T$ as a function of radius at three heights above the inlet plane: $y/d = 15$, $y/d = 45$ and $y/d = 75$. The full FGM/PDF model (solid line) and the diffusion flamelet (dashed line) are shown together with measurements (circles).
The diffusion flamelet model yields better predictions for $\dot{c}$ not just at the symmetry axis for $y/d < 60$ but also in radial direction at $y/d = 15$ and $y/d = 45$. For the temperature $T$ predictions made by the full FGM/PDF model do not deviate significantly from predictions made by the diffusion flamelet model for $y/d = 15$ and $y/d = 45$. At $y/d = 75$ predictions made by the full FGM/PDF corresponds slightly better to measurements than predictions of the diffusion flamelet model.

4 Discussion

The Sandia Flame D has been used as a first test case to prove the concept of the FGM/PDF approach for the simulation of turbulent partially-premixed combustion. The innovation of the FGM/PDF method compared to others is that it takes non-equilibrium into account by using detailed chemistry information from premixed flamelets. In highly turbulent flows it is assumed that information from premixed flamelets describes chemistry better than information from non-premixed flamelets since species are mixed very fast by turbulent eddies. The influence of turbulence has been modelled using the realizable $k, \epsilon$ turbulence model. To test the turbulence-combustion interaction of the full FGM/PDF model it has been compared with a reduced FGM/PDF version, a chemical equilibrium FGM/PDF version, a diffusion flamelet model and experimental data from literature. The reduced FGM/PDF model includes a transport equation for the reaction progress variable $\dot{c}$ but contains no turbulence-chemistry interaction for $c$. The chemical equilibrium FGM/PDF model only described the transport and turbulence-chemistry interaction for the mixture fraction $Z$.

The predictions of axial velocity and the mixture fraction made by all FGM/PDF versions agreed well, both qualitatively and quantitatively, with the diffusion flamelet model and measurements. All versions of the FGM/PDF model and the diffusion flamelet model did not predict the magnitude of the turbulent kinetic energy correctly. This is most probably caused by shortcomings of the (realizable) $k, \epsilon$ turbulence model used by all versions of the FGM/PDF model and the diffusion flamelet model. A more refined turbulence model like the Reynolds Stress Model (RSM), or using LES [18] instead of RANS (with the $k, \epsilon$ turbulence model) simulations, could yield better results since turbulence is generally predicted better.

For the mixture fraction variance $\xi$ the diffusion flamelet model gives a better prediction than the full FGM/PDF model. The overprediction of $\xi$ by all versions of the FGM/PDF model is most probably caused by a larger gradient in $Z$ in the region $20 < y/d < 60$.

The FGM/PDF models overestimate the mean reaction progress variable $\dot{c}$ by as much as 20% compared to measurements in the region $40 < y/d < 55$. This overestimation is probably due to the use of premixed flamelets instead of diffusion flamelets to describe non-premixed combustion. The sharp peak of $\dot{c}$ produces a wiggle in the reaction progress variable variance $\phi$ due to applied modelling assumptions for the production term of $\phi$.

In the upstream region of the computational domain ($y/d < 60$) where mixture fraction gradients are large the diffusion flamelet model gives a better prediction for the temperature than the full FGM/PDF model. In the downstream region ($y/d > 60$) where mixture fraction gradients are relatively small, and thus premixed combustion phenomena will dominate, the full FGM/PDF model using premixed flamelets gives a better prediction than the diffusion flamelet model. The wiggle in $\phi$ at $y/d \approx 45$ causes all profiles for interpolated variables, like temperature and species concentrations, to exhibit a similar wiggle.

It is important to notice that the full FGM/PDF and the diffusion flamelet model corresponded better to each other than any of them with the experiments. The shortcomings in modelling of influences from turbulence seem to be more limiting than shortcomings in the predictions of chemistry using either the full FGM/PDF model or the diffusion flamelet model. Results can be improved slightly without using another turbulence model by fine-tuning modelling constants in equations 8 and 10. In this study for equation 8 modelling constants have been taken equal to constants used in FLUENT [9] to facilitate a fair comparison between the FGM/PDF models and the diffusion flamelet model.

The results presented in this work show that a diffusion flame with a moderate turbulence-combustion interaction like the Sandia Flame D can be described approximately as accurate using the full FGM/PDF model as by a diffusion flamelet model. In the vicinity of the separate fuel- and oxidizer inlets ($y/d \leq 30$), where predicted turbulence intensity is relatively low, the full FGM/PDF model using premixed flamelets does not predict variables as good as the diffusion flamelet model. This was expected since due to the separate inlets and the low turbulence intensity gradients in mixture fraction are large and non-premixed combustion will dominate premixed combustion.

The conclusion can be drawn that in a non-premixed region with a moderate deviation from chemical equilibrium the full FGM/PDF model does not perform as well as a diffusion flamelet model although a reaction progress variable takes this deviation from chemical equilibrium into account. The fact that the full FGM/PDF model does not perform as good as the diffusion flamelet model is probably caused by the fact that there is no interaction...
between flamelets in the full FGM/PDF model; in non-premixed regions there is a strong diffusive interaction between different $Z$ levels.

It can be concluded that the full FGM/PDF model yields results approximately as good as established models like the diffusion flamelet model for a test case with a moderate turbulence-chemistry interaction. It is expected that the full FGM/PDF model will give better predictions than the diffusion flamelet model for turbulent flames with a higher turbulence intensity. Gradients in $Z$ will then be smaller and non-premixed combustion will not dominate premixed combustion anymore. With increasing turbulence intensity larger regions can then be described properly using the full FGM/PDF model.

References