Assumed PDF Modeling in Rocket Combustion Simulations

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Abstract

In order to account for the strong interaction between turbulence and chemistry an assumed PDF (Probability Density Function) approach is used to simulate a model rocket combustor. The reported test case is the Pennstate preburner combustor with a single shear coaxial injector. Experimental data for the wall heat flux is available for this configuration. Simulation results with and without assumed PDF approach will be analyzed and compared. Significant differences between the two calculations are expected. Moreover, the simulation with assumed PDF should be able to reproduce the measured wall heat flux more accurately.

1. Introduction

Due to the high experimental costs it is inevitable to utilize CFD (Computational Fluid Dynamics) simulations in the design process of rocket injectors and combustors. However, even the capabilities of high-fidelity approaches like LES (Large Eddy Simulation) have to be improved in order to be accurate enough, to have a quantitative influence on the injector design process [1]. Direct Numerical Simulation (DNS) approaches would yield much better results, but are computationally still more expensive and therefore restricted to the simulation of single injector near field phenomena assuming non-reacting flows or using simple combustion models. Ideally, however, a CFD tool should be able to simulate complete combustor geometries with up to several hundred injector heads including the nozzle in an acceptable timespan and at acceptable cost. Accordingly, RANS methods are still the design tools of choice in industrial applications.

Though unsteady RANS simulations have demonstrated the capability to yield quite useful results for a single shear coaxial element with gaseous propellants [2], they are not able to reproduce the strong non-linearity of the chemical source terms arising from turbulence chemistry interaction. Instead they usually treat chemistry in a "laminar" way. The use of PDF (probability density functions) methods is a promising approach to tackle this problem. It appears to be the natural choice to treat statistical fluctuations in the flowfield with probabilistic methods. The two major groups of PDF methods are the *assumed PDF* approaches and the *PDF transport equation* methods.

The more sophisticated approach, that doesn't predefine the shape of the PDF, is the solution of a PDF transport equation. It has the advantage of treating convection and finite-rate nonlinear chemistry exactly, if the PDF comprises all relevant variables. Those variables are the velocity vector for the convection and the thermochemical variables (h and Y_i) for the source term due to chemical reactions. This approach is called joint velocity-scalar PDF. However, there remain closure problems due to the fluctuating pressure gradient and due to molecular transport [3] which have to be modeled. Furthermore transported PDF approaches require extensive computational resources.

In assumed PDF methods the shape of the PDF is mathematically predefined. Thus the main focus in these methods is to find functions that are as simple as possible from a mathematical point of view but flexible enough to be able to approximate the realistic PDF shapes, observed in experiments, with high accuracy. Due to the comparatively low computational costs, assumed PDF methods are widely used and have proven the capability to produce useful results in a wide variety of combustion conditions [4, 5].

2. Numerical Code

For the simulation the scientific TASCOM3D (Turbulent All Speed Combustion Multigrid 3D) code is used. The code solves the conservation equations for mass, momentum, energy and species as well as equations for turbulence closure. Several two-equation turbulence models are implemented in the code. However, the presented results are obtained with

the q-ω-model proposed by Coakley et al. [6]. If the assumed PDF module is activated, two additional equations for the temperature variance and the variance of the sum of the species mass fractions have to be solved. The complete set of equations in three-dimensional conservative form can be written as

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial (\mathbf{F} - \mathbf{F}_v)}{\partial x} + \frac{\partial (\mathbf{G} - \mathbf{G}_v)}{\partial y} + \frac{\partial (\mathbf{H} - \mathbf{H}_v)}{\partial z} = \mathbf{S}\,, \tag{1}$$

with the vector of conservative variables

$$\mathbf{Q} = \left[\bar{\rho}, \bar{\rho}\tilde{u}, \bar{\rho}\tilde{v}, \bar{\rho}\tilde{w}, \bar{\rho}\tilde{E}, \bar{\rho}q, \bar{\rho}\omega, \bar{\rho}\sigma_T, \bar{\rho}\sigma_Y, \bar{\rho}\mathbf{Y}\right]^T \quad . \tag{2}$$

The variables in the variable vector $\mathbf{Q}$ are the density $\bar{\rho}$ (averaged), the velocity components (Favre averaged) $\tilde{u}$, $\tilde{v}$ and $\tilde{w}$, the total specific energy $\tilde{E}$, the turbulence variables $q = \sqrt{k}$ and $\omega = \epsilon/k$ (where k is the kinetic energy and ϵ the dissipation rate of k), the variance of the temperature σ_T and the variance of the sum of the species mass fractions σ_Y. The vector $\mathbf{Y}$ contains the species mass fractions $\tilde{Y}_i$ for $i = 1, 2, \ldots, N_k - 1$ and N_k is the total number of gaseous species. Since the set of equations includes the conservation of mass, $N_k - 1$ species transport equations have to be solved, only. In Eq. (1) the vectors $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{H}$ specify the inviscid fluxes in x-, y- and z- direction, $\mathbf{F}_v$, $\mathbf{G}_v$ and $\mathbf{H}_v$ the viscous fluxes, respectively.

The assumed PDF approach uses mathematically predefined probability density functions for the temperature and the species mass fraction. A widely used approach for the temperature PDF P_T is the clipped Gaussian distribution.

$$\begin{aligned} P_T\left(\hat{T}\right) = \frac{1}{\sqrt{2\pi\sigma_T}} \exp\left(-\frac{\left(\hat{T} - \tilde{T}\right)^2}{2\sigma_T}\right)\left(\theta(\hat{T} - T_{min}) - \theta(\hat{T} - T_{max})\right) \\ + A_l\delta(\hat{T} - T_{min}) + A_r\delta(\hat{T} - T_{max}) \quad . \end{aligned} \tag{3}$$

The constants A_l and A_r correspond to the clipped parts and determine the magnitude of the delta pulses in order to satisfy the normalization condition.

As for the composition PDF Girimaji [7] proposed a multi-variate β-PDF

$$P_Y\left(\hat{Y}_1, ..., \hat{Y}_{N_k}\right) = \frac{\Gamma\left(\sum_{m=1}^{N_k} \beta_m\right)}{\prod_{m=1}^{N_k} \Gamma\left(\beta_m\right)} \left[\delta\left(1 - \sum_{m=1}^{N_k} \hat{Y}_m\right) \prod_{m=1}^{N_k} \hat{Y}_m^{\beta_m - 1}\right] \tag{4}$$

for the sum of the species mass fractions, where

$$\beta_m = \tilde{Y}_m B, \quad B = \left[\frac{\sum_{m=1}^{N_k} \tilde{Y}_m\left(1 - \tilde{Y}_m\right)}{\sigma_Y} - 1\right], \quad \sigma_Y = \sum_{m=1}^{N_k} \widetilde{Y_m''^2} \quad . \tag{5}$$

The delta function is needed so that the PDF fulfills the normalization condition. Though the neglection of the full matrix of variances and covariances means a loss of information, the consideration of only the trace of the matrix, leads to a significant reduction of computing time. When dealing with detailed chemistry the number of components N_k becomes quite large so that the solution of $n = m^2 + m/2$ transport equations ($m = N_k - 1$) becomes impossible for practical simulations. This assumed PDF approach has proven to yield accurate results for a variety of flames [4, 5].

In TASCOM3D chemical reactions are treated fully coupled with the fluid motion by a finite-rate chemistry approach, where the reaction rate k_r is obtained by the Arrhenius law

$$k_r = A_r T^{n_r} \exp\left(\frac{-E_r}{R_m T}\right) \tag{6}$$

with the temperature T and the gas constant R_m. The parameters A_r, n_r and E_r are available from literature for a variety of reaction mechanisms. As for the simulations presented here, the hydrogen oxidation scheme of Ó Conaire *et al.* [8] with 19 reactions and 8 species is used, because it is also well validated for the regime of elevated pressures.

Equation (1) is solved on structured multi-block meshes via an implicit Lower-Upper Symmetric Gauss-Seidel (LU-SGS) [9] FV-algorithm. Due to recent work [10] the spatial discretization is of up to fifth order, whereas the temporal resolution is of up to third order. The code has been parallelized through MPI (Message Passing Interface) and is optimized to run on array processor architectures. *TASCOM3D* has been validated by a variety of combustion simulations ranging from subsonic [4] to supersonic [5] flows.

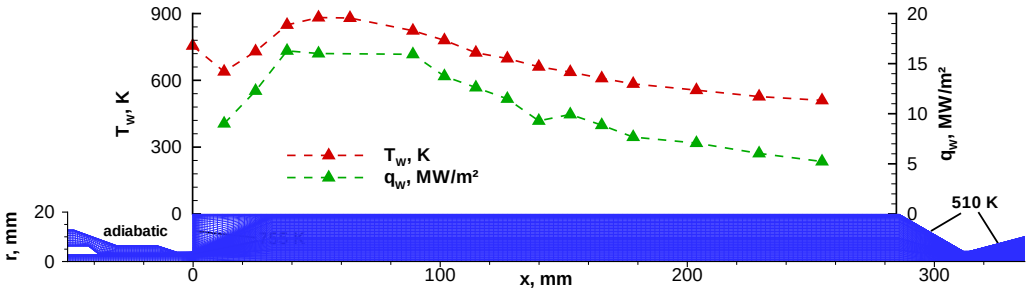

Figure 1: Computational domain, measured wall temperatures and measured wall heat fluxes for the PennState preburner combustor.

3. Test Case

Within the framework of the program "Focused Validation Data for Full Flow Staged Combustion (FFSC) Injectors" funded by NASA an GO2/GH2 single element combustor, the so called PennState preburner combustor, was examined at the Cryogenic Combustion Laboratory at the Pennsylvania State University. The specific interest in FFSC cycle engines arises from their simplicity and increased thrust to weight ratio, relative to other closed cycle engines. The experiment reported by Marshall *et al.*[11] was designed to characterize the chamber wall heat transfer. Therefore the circular combustion chamber was equipped with a large amount of Gordon type heat flux gauges and coaxial thermocouples. The axial positions of the temperature and heat flux measurements are illustrated in Fig. 1. The chamber diameter is 38.1 mm and its length 285.75 mm. Two upstream preburners produce oxidizer-rich and fuel-rich gases, respectively. The oxidizer-rich gas is fed to the combustion chamber through the inner tube of the coaxial injector with a diameter of 5.26 mm and is recessed 0.43 mm with respect to the combustion chamber face plane. The annular fuel feed has an inner diameter of 6.30 mm and an outer diameter of 7.49 mm. The operating conditions of the PennState preburner combustor are summarized in Tab. 1. It has to be noted that the GO_2 and GH_2 mass flow rates to the preburners were measured. Together with the measured preburner and combustion chamber pressures the properties downstream of the preburners were calculated using the NASA chemical equilibrium code CEA. More details on the derivation can be found in [12]. The PennState preburner combustor test case has recently been of great interest for model validation and was simulated using a variety of modeling approaches [1, 2].

The simulations are performed as unsteady 2D axisymmetric calculations on the computational domain illustrated in Fig. 1 with approximately 215 000 volumes. Wherever possible, the measured temperatures are set as boundary conditions. The injector post tip wall is assumed as isothermal with a temperature of 755 K. For the combustion chamber wall a temperature distribution corresponding to a least squares fit of the measured data points is set as boundary condition. The nozzle is water-cooled and has a temperature of 511 K. All other walls are assumed to be adiabatic. The inflow conditions correspond to the values in Tab. 1.

		Oxidizer Preburner	**Fuel Preburner**
pressure	MPa	5.85	6.50
temperature of products	K	700	811
O_2 mass flow in products	kg/s	$8.55 \cdot 10^{-2}$	-
H_2 mass flow in products	kg/s	-	$1.33 \cdot 10^{-2}$
H_2O mass flow in products	kg/s	$4.98 \cdot 10^{-3}$	$1.98 \cdot 10^{-2}$
		Main Chamber	
pressure	MPa	5.42	

Table 1: Operating conditions of the PennState preburner combustor test case.

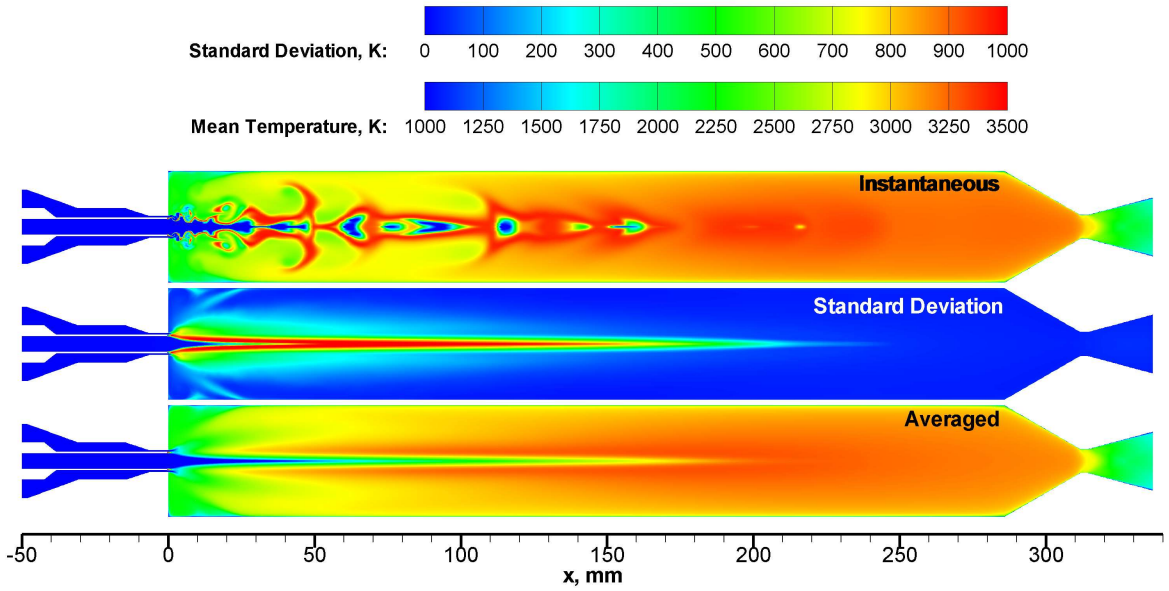

Figure 2: Temperature results of the simulation without turbulence-chemistry interaction. From top to bottom an arbitrary instantaneous temperature field, the standard deviation and the mean temperature are illustrated.

4. Preliminary Results

So far unsteady calculations of the PennState preburner combustor test case without assumed PDF module have been performed. The results for the temperature contours are shown in Fig. 2. The contour plot at the top shows an arbitrary instantaneous temperature distribution of the unsteady simulation with fifth order spatial discretization. Below the standard deviation and the averaged temporal data of the same calculation are shown. The instantaneous graph clearly indicates the highly unsteady flow features in the near-injector region causing a strongly corrugated flame. This is also evident in the region of very high standard deviations of up to 1000 K, that originates from the oxidizer post tip stretching towards the combustor center line where it reaches far into the chamber. Further downstream the injector the turbulent features decrease gradually. Thus the instantaneous and averaged temperatures coincide quite well in the last third of the combustor. Near the injector, however, there is a large region with high standard deviations from the mean temperature caused by the unsteadyness of the flame front.

Figure 3 shows the measured heat flux data in comparison with the simulation result. The shape of the distribution as well as the position and the magnitude of the maximum wall heat flux are reproduced quite accurately by the simulation. The maximum heat flux is only slightly underpredicted by around 1.5 MW/m^2, which is less than 10%. Nevertheless it has to be mentioned, that the initial rise in heat flux is shifted downstream by approximately 10 mm compared to experimental data.

Simulations that consider turbulence-chemistry interaction by means of an assumed PDF approach are still ongoing. They will be analyzed and compared to the presented simulation as well as the experimental data.

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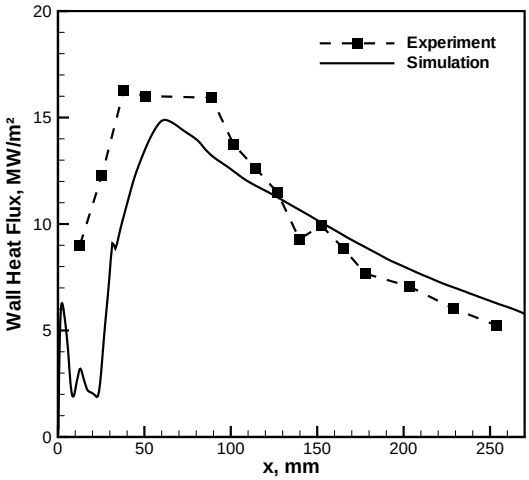

Figure 3: Comparison between the measured wall heat flux and the simulation without assumed PDF modeling.

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