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Velocity-Composition Probability Density Function Modelling for Non-Premixed Turbulent Flame DNS

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Abstract

The velocity-composition joint probability density function (VC-TPDF) model was implemented in a Reynolds-averaged Navier-Stokes context, validated, and tested a posteriori against results from a direct numerical simulation (DNS). The VC-TPDF transport was modelled using the simplified Langevin model (SLM) for the velocity statistics. A validation was first performed against analytic solutions from a mean scalar gradient test case and an excellent agreement was observed. Comparisons were then made with a direct numerical simulation (DNS) test case. The DNS scenario was a non-premixed, turbulent, syngas jet flame, exhibiting local extinction and re-ignition. The Favre-averaged DNS data were compared with the VC-TPDF model and previous modelling using the composition joint probability density function model. The SLM-based VC-TPDF model was able to qualitatively capture the extinction and re-ignition behaviour, however, incorrect jet-spreading was observed. An ad-hoc adjustment of the turbulence production term in the SLM was performed to investigate the jet spreading. It was found that by artificially increasing the turbulence generation, that the correct jet-spreading behaviour could be produced in mean quantities, however, this also caused spurious production variance and so is not a feasible solution. It is speculated that the incorrect jet spreading observed is due to insufficient production of turbulence in the SLM, which may be attributed to assumptions such as isotropy which neglects the anisotropic production of turbulence that would occur in a shear driven jet configuration. It is proposed that a generalised Langevin model is required to correctly model the jet case.

Introduction

Transported probability density function (TPDF) methods offer a flexible framework for modelling turbulent combustion [2,5]. TPDF methods are general, due to making few assumptions, and permit an exact closure of the chemical source term [2,5]. Variants of the TPDF methods include the composition (C-TPDF), and velocity-composition (VC-TPDF) transported probability density function models, which differ by their degree of closure and the number of transported variables. The C-TPDF model solves transport equations of scalars only, such as species mass fractions and enthalpy, whereas the VC-TPDF model also solves for the velocity [2,5]. In C-PDF, turbulent transport of scalars must be modelled, usually by assuming gradient transport, while turbulent transport of scalars is an outcome of the VC-PDF model.

In previous work by some of the present authors [3], a Reynolds averaged Navier-Stokes (RANS) implementation of the C-TPDF model was tested in comparison to direct numerical simulations (DNS) of non-premixed temporal jet flames burning syngas [1] and ethylene [4] at various levels of turbulence. The focus of that paper was on the validation and comparison of various mixing sub-models. The present study provides an extension of that work, wherein a VC-TPDF model is implemented in the same computational framework.

Two test cases were considered: a mean scalar gradient (MSG) case and a non-premixed turbulent jet case (syngas case M from [1,4]). The MSG test case was selected to provide an analytical solution with which to verify the VC-TPDF implementation. Case M (a case with moderate levels of extinction) was selected to compare the performance of the VC-TPDF model against the DNS and C-TPDF baselines.

The VC-TPDF model was implemented with a hybrid particle-mesh domain and a time-splitting method. Model equations for the position, X^*, velocity, V^*, and compositions, φ^*, are solved for each particle according to Eqns. 1→ 3:

$$dX^* = V^* dt \tag{1}$$

$$dV^* = -\frac{1}{\bar{\rho}}\frac{d\bar{p}}{dy}dt - \left(\frac{1}{2}+\frac{3}{4}C_0\right)\tilde{\Omega}\left(V^* - \tilde{V}\right)dt + \sqrt{C_0 C_1 \tilde{\varepsilon}}\,dW \tag{2}$$

$$d\phi^* = [M^*]dt + [R^*]dt \tag{3}$$

where $\bar{P}$ is the mean pressure field, $\tilde{\Omega}$, is the turbulent mixing frequency, $\tilde{\varepsilon}$, is the turbulent dissipation rate, and these values are obtained directly from the DNS for case M. [M^*] represents the effect of molecular mixing and is implemented here with the interaction by exchange with the mean (IEM) mixing model [9]. [R^*] represents the chemical reaction and is evaluated in an identical manner to the DNS [1] for case M, and is set to zero for the non-reacting MSG case.

Equation 2 is the simplified Langevin model (SLM) [6,7] which models the velocity statistics in the VC-TPDF method and is the focus of this study. The terms on the right hand side of Eqn. 2 represent the: pressure gradient force, which is primarily due to heat release; the relaxation towards the mean velocity, which is the turbulence dissipation mechanism; and the stochastic generation of turbulence, where dW is an increment of a Wiener process. Here two model constants are used: C_0 is the standard model constant, and C_1, which is normally unity, was introduced to vary the production of turbulence in an ad hoc manner.

The results presented in this paper for the non-premixed turbulent jet case use 4000 number of particles per cell (N_{PC}), 384 number of cells (N_{CELL}) and a time step (t_{STEP}) of 5×10^{-8} s. The number of grid points in the DNS input data is 1000. Results presented for MSG test case use 1000 N_{PC}, 96 N_{CELL} and t_{STEP} of 1×10^{-7} s.

Verification

To validate the VC-TPDF model, a MSG test was conducted, as per Ref. [8]. In this simple test case, turbulent transport and mixing is considered for a non-reacting scalar having a specified gradient, enforced within a finite size domain having a jump periodic boundary condition for the scalar. The scalar variance (K_ϕ) and scalar flux values (F_ϕ) were compared with the theoretical results, which evolve according to Eqns. 4 and 5:

$$K_\phi(t) \equiv \frac{\langle Z^2 \rangle}{(G\sigma^2 T_L)} \equiv \frac{4}{(2c_\phi + 1)^2 - 1} \quad (4),$$

$$F_\phi(t) \equiv \frac{\langle UZ \rangle}{(G\sigma T_L)^2} \equiv -\frac{1}{1 + c_\phi} \quad (5),$$

here Z is the mixture fraction, U is the velocity, C_ϕ is the mixing constant, and G, σ and T_L are normalization constants as described in Ref. [8]. In the our case the values of normalization constants are: $G = 100\ \text{m}^{-1}$, $T_L = 1$ s , and $\sigma = 0.1\ \text{ms}^{-1}$.

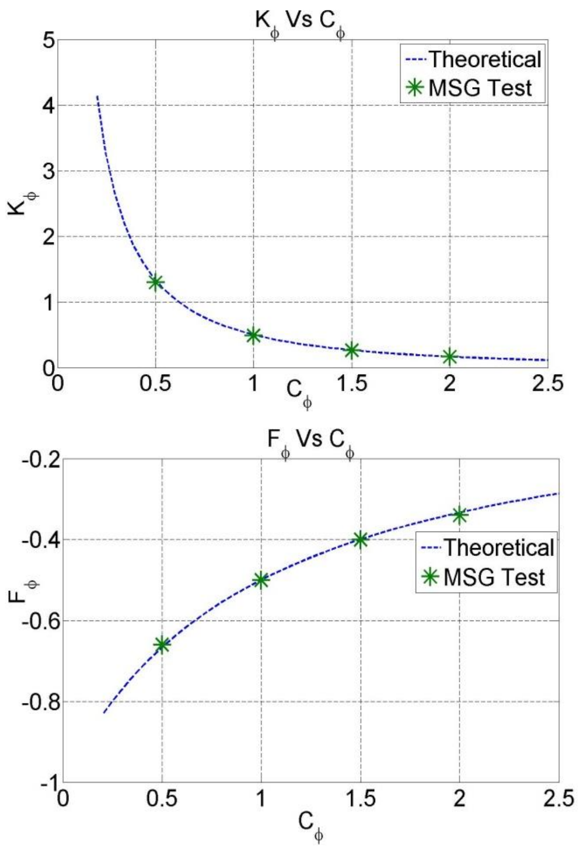


Figure 1 Mean scalar gradient scalar flux (top) and scalar variance (bottom).

Figure 1 shows the results of the verification. An excellent agreement is observed between the VC-TPDF results and the theoretical values for both the scalar flux and the scalar variance. This provides confidence that the VC-TPDF method was correctly implemented.

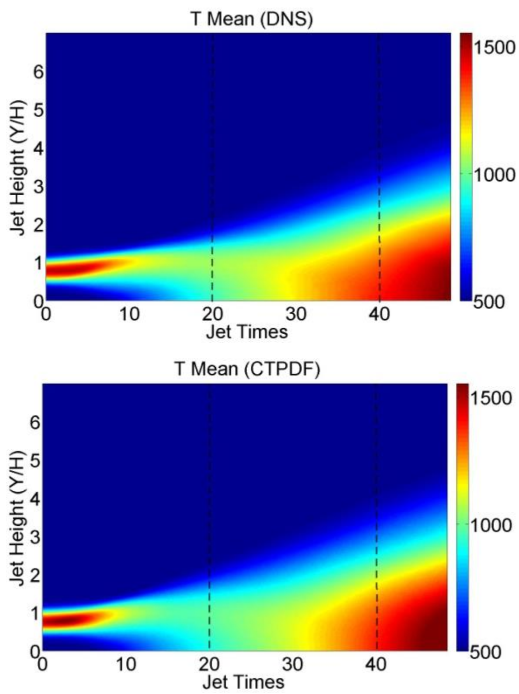
Results

Two set of results are presented in this paper: one with the standard value of C_0=2.1 and C_1=1.0 (standard constants) [6,8] , and the other with C_0=2.1 with C_1=1.9 (adjusted constants). Model results using the standard coefficients will be referred to as VC-TPDF$_{ST}$, model results using the adjusted coefficients will be referred to as VC-TPDF$_{AD}$.

Figure 2 shows the evolution of the mean temperature for the DNS and the C-TPDF and VC-TPDF$_{ST}$ models. While the VC-TPDF$_{ST}$ model produces qualitatively correct extinction and re-ignition behaviour, the jet-spreading is clearly incorrect.

The mean mixture fraction, Z, and root mean square (RMS) mixture fraction, Z_{RMS}, is shown in Figs. 3 and 4, respectively, for the DNS, C-TPDF, VC-TPDF$_{ST}$, and VC-TPDF$_{AD}$ at 20 and 40 jet times. The Z profile confirms that the VC-TPDF$_{ST}$ constants produce insufficient jet-spreading. The adjusted constants produce a result comparable to the C-TPDF model. Although the adjusted constants produce the correct jet spreading, the Z_{RMS} profile reveals that there is spurious production of variance within the co-flow.

To investigate this further, the mean velocity, V, and RMS velocity, V_{RMS}, are presented in Figs. 5 and 6, respectively, for the DNS, VC-TPDF$_{ST}$, and VC-TPDF$_{AD}$ at 20 and 40 jet times. At 20 jet times, neither set of coefficients produces the correct V profile. At 40 jet times, the VC-TPDF$_{AD}$ result is accurate within the jet, but overestimated in the co-flow, whereas the opposite is true for the VC-TPDF$_{ST}$ results. In terms of the V_{RMS} profile, at 20 jet times the standard coefficients are close to the DNS result, but the adjusted coefficients over-estimate V_{RMS}. At 40 jet times, both sets of coefficients overestimate V_{RMS}, but the VC-TPDF$_{ST}$ result is much closer to the DNS.



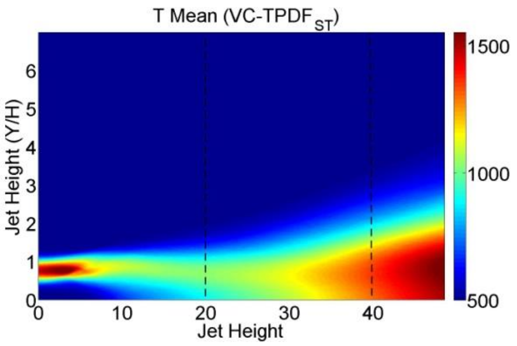


Figure 2. Mean temperature profile for DNS, C-TPDF and VC-TPDF$_{ST}$ models. The dotted lines mark the 20 and 40 jet times position.

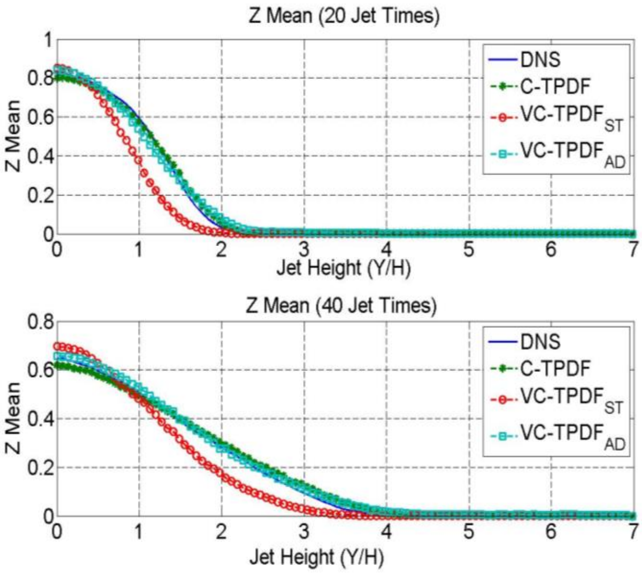
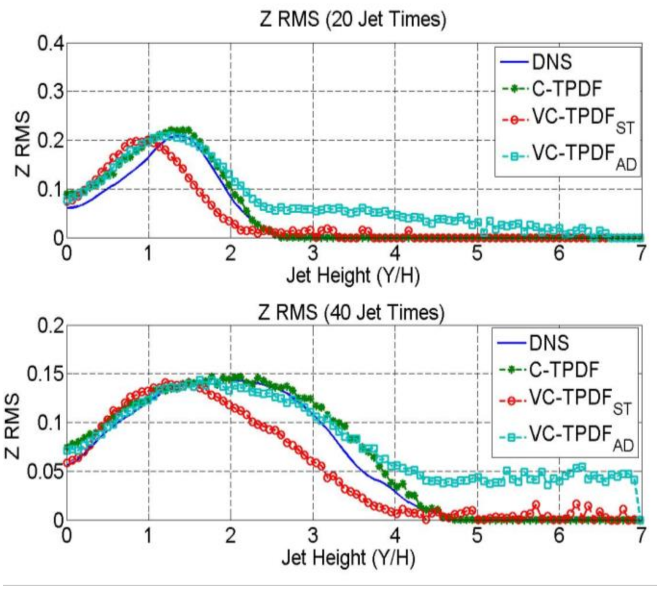


Figure 3. Mean mixture fraction profile at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models.



Fiugre 4. RMS mixture fraction at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models

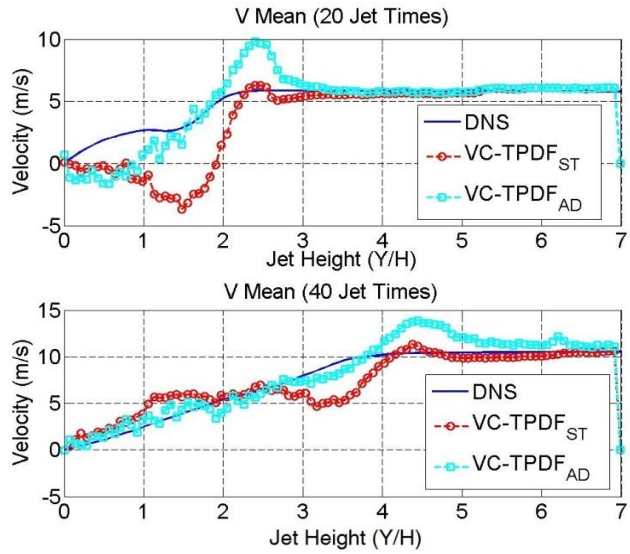


Figure 5. Mean velocity profile at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models.

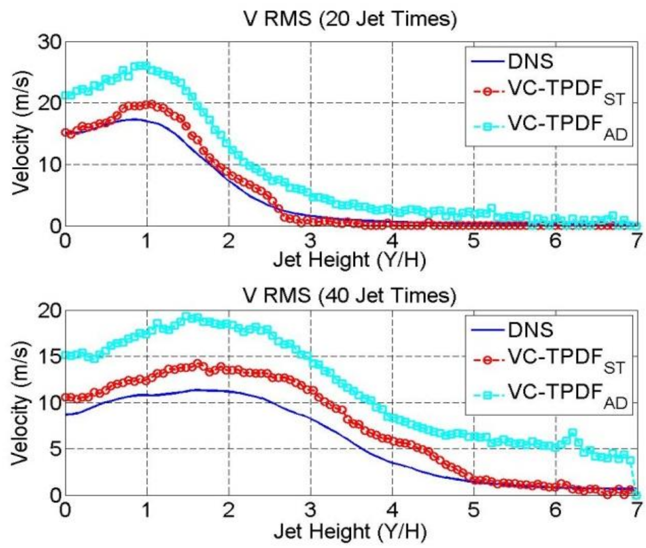


Figure 6. RMS velocity profile at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models.

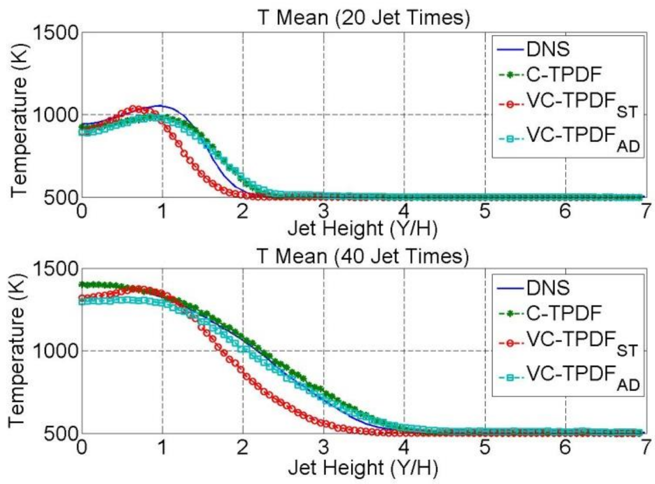


Figure 7. Mean Temperature statistics at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models.

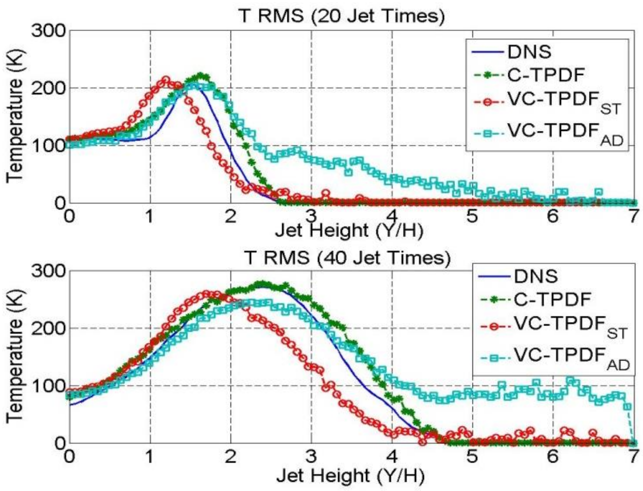


Figure 8. RMS temperature profile at 20 and 40 jet times for DNS, C-TPDF and VC-TPDF models.

Discussion

Adjustment of the model constant C_0 was unable to produce the correct jet-spreading behaviour. This motivated the introduction of the constant C_1, in order to investigate the effect of increasing the turbulence production in the SLM in an ad-hoc manner.

It was possible to adjust the model constants such that the jet-spreading was broadly correct in the mean. However, by adjusting the model constants, spurious production of scalar variance was observed in the co-flow. Additionally, the adjusted constants caused the velocity fluctuations to increase throughout the domain, to values approximately 1.5 to 2.0 times greater than that of the DNS.

The necessity to perform an ad-hoc variation of C_1 therefore suggests that there is an insufficient production of turbulence in the SLM model. The assumptions in the SLM model are likely at fault. For example, the assumption of isotropy may be resulting in an under-prediction of turbulence since the shear generated turbulence of the jet is strongly anisotropic.

It is therefore necessary to implement the generalised Langevin model (GLM), which contains fewer simplifying assumptions.

Conclusions

A VC-TPDF model was implemented in a RANS context. The velocity statistics were obtained using the SLM model, which assumes isotropic turbulence.

The VC-TPDF model was validated in the configuration of a mean scalar gradient, for which analytical solutions are available. An excellent agreement between the model and the theoretical solution was obtained, providing confidence that the model was correctly implemented.

The VC-TPDF model was then tested in the case of a non-premixed turbulent jet flame with a syn-gas fuel. Using the standard model constant value of C_0 = 2.1, insufficient spreading of the jet was observed, although the qualitatively correct extinction and re-ignition behaviour was obtained.

A second model constant C_1 was introduced into the turbulence production term of the SLM model, to investigate the behaviour of the jet spreading in an ad-hoc manner. It was found that by setting the model constants to C_0=2.1 and C_1=1.9, that the correct jet spreading was produced. However, this is not a feasible solution for the VC-TPDF implementation; it produced spurious variance of scalar quantities in the co-flow and greatly overestimated velocity fluctuations throughout the domain.

The ad-hoc variation of C_1 indicates that there is insufficient production of turbulence in the SLM model. Since the SLM model assumes isotropy, and the shear-driven turbulence of the jet is strongly anisotropic, it is speculated that the problem is the absence of anisotropic turbulence production terms in the velocity equation.

An implementation of the generalised Langevin model, which includes anisotropic turbulence production terms, is proposed for future work.

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