Consistent turbulence modeling in a hybrid LES/RANS PDF method for non-premixed flames

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Abstract

A hybrid LES-RANS PDF method for non-premixed flames, based on the transport equation of the PDF conditioned on mixture fraction, is developed, in which the turbulent transport of the mixture fraction in LES is combined with the conditioned turbulent reaction in RANS-PDF. The RANS Lagrangian composition PDF is performed using velocity field and the turbulent quantities from the LES solution. However, LES/RANS coupling create a consistency issue due to the intrinsic theoretical differences of the two models. In particular, the turbulent viscosity and turbulence frequency calculated in LES as subgrid values can not be directly used within a RANS simulation. An algebraic model to establish consistency between LES and RANS has been used in this work to simulate the Sandia D flames. Moreover, the new implementation of whole algorithm in OpenFOAM is presented.

Introduction

Coupling the LES (Large Eddy Simulations) with RANS (Reynolds-Averaged Navier Stokes) is becoming an interesting procedure for many different CFD applications. The goal is to combine the advantages of the two methods, reducing the computational effort. The LES is known to be able to better represent large-scale turbulent flow structures, which are controlled by the geometry of the flow configuration and which mainly characterize the global turbulent mixing. Small scale turbulent motions and mixing can be expected to behave more universally and thus are more amenable to model. However, LES finds its limitations in the high computational requirements for fine mesh and time resolution [1]. Compared to LES, RANS simulations are by a factor 10 to 100 less computational costly [2], but show their shortcomings when are applied to unsteady or complex flows, resulting in an overprediction of eddy-viscosity and an over-damping of the unsteady motions [3].

Turbulent reacting flows require an additional modelling effort due to the non-linear interactions between turbulence and chemistry. Probability Density Function (PDF) methods, firstly proposed by Pope in [4], have the main advantage to represent the non-linear chemical sources in closed form, without any modeling assumptions. Therefore the full range of available and sophisticated chemistry mechanisms can in principle be directly applied. Past works have demonstrated the ability of PDF methods to simulate non-premixed flames [5, 6]. The PDF is represented by an ensemble of stochastic particles, whose properties evolve according to stochastic differential equations and exhibit the same JPDF as the one obtained solving the JPDF transport equation. Moreover, in this method the computational effort increases only linearly with the number of composition variables, allowing to use also complex kinetic schemes. In joint composition-PDF methods a transport equation for PDF of reacting scalars is solved by the Monte Carlo (MC) method, while the effects of turbulent transport and molecular mixing have to be modeled.

Filtered density functions (FDF) or filtered mass density functions (FMDF) can be used to extend the TPDF concept from RANS to LES [7]. A large number of particles has to be used in each cell to build a representative FDF, requiring high computational effort [8]. An alternative "sparse" Lagrangian FDF method has been formulated in [9, 10]. In this method fewer particles than the grid cells are used to represent the composition-PDF. The computational costs are two to three orders of magnitude smaller than that required in a classical LES-FDF simulation, while the results are comparable.

Different from the existing concepts, in this work the developments and a new implementation of the hybrid LES/ RANS-Lagrangian PDF method, firstly described in [1], are presented. By introducing a transport PDF equation conditioned on the mixture fraction, the modelling of the transport PDF equation has been split into the modelling of the transport of the mixture fraction and the modelling of the transport of the species conditional PDF. This hybrid method provides a combination of the detailed flow field representation from LES and the general chemistry model from PDF method. In non-premixed combustion,

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the hybrid method firstly conducts a LES steady flamelet simulation, which will supply mean velocity and the turbulence fields to the composition RANS-PDF. Then by applying Bayes theorem, in the RANS-PDF simulation the chemical species are evaluated based on both the RANS conditional PDF and the PDF of the mixture fraction taken from the related LES simulation. In this way the hybrid method combines the turbulence model of the LES and the chemistry model of the RANS-PDF. Most importantly in hybrid method, the computational cost of the chemistry model is kept within the RANS context. The whole algorithm of the hybrid method has been implemented within the open-source CFD tool OpenFOAM [11]. A fully consistent coupling method is applied to transfer the mean velocity and other required turbulence quantities from LES to RANS, based on the ensemble average LES quantities and an algebraic turbulent model. To validate the coupled hybrid method numerical simulations on Sandia flame D [12] are shown.

Transport equation of the conditional composition PDF

In turbulent diffusion flames, reactive scalars Y_i depend on mixture fraction f, which describes the mixing between fuel and oxidizer [13]. With this assumption, the conditional statistics of reactive scalars can be separated from small scale turbulence. Following the PDF theory [4], from the transport equation of the fine-grained PDF, we derive the transport equation for the PDF of the reaction scalars, conditioned on mixture fraction [14], $P_f = P(\mathbf{Y}|f;\mathbf{x},t)$

$$\begin{aligned}\frac{\partial}{\partial t}\left(\overline{\rho}\tilde{P}_f\right) + \nabla\left(\overline{\rho}\tilde{u}\tilde{P}_f\right) + \frac{\partial}{\partial\psi_i}\left(\overline{\rho}\langle W_i|\psi=f\rangle P_f\right) \\ = -\frac{\partial^2}{\partial\psi_i\partial\psi_j}\left(\overline{\rho}\langle D(\nabla Y_i\nabla Y_j)|\psi=f\rangle\tilde{P}_f\right) \\ -\nabla\left(\overline{\rho}\langle\nu''|\psi=f\rangle\tilde{P}_f\right.\end{aligned} \quad (1)$$

where ψ_i are the random variables, W_i the species chemical reaction rates and $D_i = D$ the diffusion coefficients similar for all the species. The first two terms of Eq. (1) represent the rate of change of conditional PDF $\tilde{P}_f$, following a particle moving with mean velocity $\tilde{u}$; the third term represents the effect of the chemical reactions. All these terms are in closed form, whereas the terms on the right-hand side have to be modeled. The first term on the right-hand side represents the transport in composition space due to molecular diffusion and is modeled by a stochastic mixing model. The final term represents the transport in physical space due to the velocity fluctuations and is modeled with the turbulent diffusivity approach. The high Reynolds number hypothesis allows neglecting molecular diffusion effects on turbulent transport [15]. The Eq. (1) has $N_\Phi + 4$ independent variables: N_Φ composition variables, spatial coordinates and time. The solution of this equation with a finite-difference method is computationally prohibitive for the high number of variables. Since the Eq. (1) has the same form of the joint PDF transport equation, in principle the MC-method, used by [4], can be also used to solve the conditional PDF.

In this work we follow the approach proposed in [14]: the MC-method is used to obtain the unconditional joint PDF in RANS context and then the conditional PDF is obtained with Bayes' theorem. We assume to know for a specific fluid problem the stationary joint PDF of the reacting scalars, $P(\mathbf{Y})$, which consists of mixture fraction, species mass fraction and enthalpy. The conditional PDF can be bijectively obtained using Bayes' theorem [16]

$$P_f = \frac{P(\mathbf{Y})}{P(f)} \quad (2)$$

The Eq. (2) provides a solution for conditional PDF P_f, which has to be equivalent to the PDF obtained solving the Eq. (1). In this way it is possible to determine the unconditional PDF using the standard RANS-PDF method and then to obtain the conditioned values. The closure with LES is established by using Bayes' theorem again, with the mixture fraction PDF $P(f)$ obtained from LES

$$P^*(\mathbf{Y}) = P_{f,MC}\, P_{LES}(f) \quad (3)$$

The advantage of this approach is that the PDF transport equation can be decomposed in a part describing the transport of mixture fraction, extracted from LES, which contains turbulent informations, and another part representing the transport of species PDF conditioned on mixture fraction, obtained with the RANS-TPDF simulation.

Hybrid LES RANS-TPDF model

The hybrid method is divided into two parts: firstly an Eulerian LES, based on the Favre filtered transport equations for mass, momentum and mixture fraction, is performed; subsequently, a Lagrangian RANS composition-PDF is carried out. In LES the species mass fractions, density and temperature are obtained using a steady laminar flamelet model as combustion model. The sub-grid distribution of the mixture fraction is described by a presumed $\beta-$PDF. The mass weighted average mixture fraction PDF, $P_{LES}(f)$, required by Eq. (3), is reconstructed from the LES solution using a large number of samples.

In RANS-TPDF, the particle evolution is governed

by the following stochastic differential equations [4]

$$dx_i^{(p)} = \big(\tilde{u_i} + \frac{1}{\overline{\rho}}\frac{\partial}{\partial x_i}(\rho D_{eff})\big)dt + \sqrt{2D_{eff}}dW_i \quad (4)$$

where $x_i^{(p)}$ is the position of the stochastic particle p in physical space, $\tilde{u_i}$ the velocity, ρ the density and dW_i the stochastic Wiener increment. The effective diffusion coefficient, $D_{eff} = D + D_t$, includes also the turbulent diffusion D_t, which is related to the viscosity through the turbulent Schmidt number. In Eq. (4) the required mean velocity, density and turbulent diffusivity quantities are extracted from the LES simulation. The procedure employed to share the LES quantities into the RANS context is presented in the following section.

The modelling of the unclosed molecular diffusion term is performed with the Modified Curl's mixing method (MCL), which allows relatively simple implementation, respecting the requirement of localness in physical space [17]. Due to molecular diffusion the particles change their composition by mixing with neighbouring particles. Given two mixing particles, i and j, randomly selected, with different weights, m_i and m_j, the scalar compositions after the mixing are

$$\begin{aligned}\phi_i(t+\Delta t) &= \phi_i(t) + \alpha\frac{m_j}{m_i+m_j}(\phi_j(t) - \phi_i(t)) \\ \phi_j(t+\Delta t) &= \phi_j(t) + \alpha\frac{m_i}{m_i+m_j}(\phi_i(t) - \phi_j(t))\end{aligned} \quad (5)$$

where α is a random number selected in the range $[0, 1]$.

LES/RANS PDF consistency

In order to build a fully consistent hybrid method, the mean velocity field and turbulence quantities, required by Lagrangian RANS simulation, are evaluated from the LES solution. Ensemble averages of the LES flow field have been calculated using a large number of samples and stored after a statistically stationary solution is obtained. From N_s instantaneous velocity samples $\tilde{u_i}^r(x_i, t)$, we obtain, according to [18],

$$\begin{aligned}\langle\tilde{u_i}\rangle &= \frac{\sum_{r=1}^{N_s}\tilde{u_i^r}}{N_s} \\ \left\langle \tilde{u_i}''^2 \right\rangle &= \frac{\sum_{r=1}^{N_s}\tilde{u_i^r}^2}{N_s} - \langle\tilde{u_i}\rangle^2\end{aligned} \quad (6)$$

the ensemble averaged LES velocity field and squared velocity resolved fluctuations, respectively, which correspond to RANS quantities.

The next consistency issue deals with the turbulent variables. A simple algebraic model is proposed for the RANS turbulent kinetic viscosity, according to a dimensional analysis,

$$\nu_{t,RANS} = C_k l_{mix}\sqrt{k_{t,res}} \quad (7)$$

where C_k is a new model constant ($C_k = 0.3$ is used here), $k_{t,res} = \frac{1}{2}\sum_i\left(\left\langle\tilde{u_i}''^2\right\rangle\right)$ the LES resolved turbulent kinetic energy and l_{mix} the turbulent length scale.

From the self-similar solution of a free round jet [19], the turbulent length scale is estimated as a mixing length, proportional to the width of the shear layer:

$$l_{mix} = \frac{1}{5}\alpha(x + \frac{5}{2}D) \quad (8)$$

where α, x, and D are the mixing-length coefficient, characteristic of the flow configuration ($\alpha = 0.08$ for round jet), the axial distance from the nozzle and the nozzle diameter, respectively.

The mixing frequency ω, which gives the mixing time scale for the micromixing is obtained as

$$\omega = \frac{C_\mu k_{t,res}}{\nu_t} \quad (9)$$

with $C_\mu = 0.9$ as in the $k-\epsilon$ model [20].

Numerical implementation

The hybrid solver involves two separate components. The LES solver is based on a Eulerian grid using a finite-volume-based discretization. The RANS-PDF solver is based on a Lagrangian scheme using a coarser grid than LES.

LES generally requires a grid resolution one order of magnitude larger than RANS method. When species conditioned of mixture fraction vary slowly in space, there is no need to use identical meshes in RANS-PDF and LES simulations. A coarser RANS grid allows to reduce the computational demand, exploitable for detailed chemical models. Both solvers are implemented in the open-source code OpenFOAM [11].

LES solver

The LES simulation is performed with the flameletFoam solver [21]. The turbulence on the subgrid scales is modeled with the algebraic Smagorinsky model. The velocity fluctuations at the fuel inlet are simulated using a random noise boundary condition. Species mass fractions values are stored in pre-processed flamelet tables, integrated with a presumed $\beta - PDF$, as function of the mixture fraction $\tilde{f}$, mixture fraction variance $\tilde{f''^2}$ and scalar dissipation rate $\tilde{\chi}$. The finite volume scheme provides the input values to interpolate the tables.

The calculation of a space-averaged $\beta-$PDF $P_{LES}(f)$,

required in the Eq.(3) has been included in the solver.

RANS-PDF solver

The RANS-PDF Lagrangian solver represents an extension of Ge's work in [10]. Stochastic particles are initialized in the domain with a weight corresponding to the mass flux in the cell. The particles move in the domain according to Eq.(4), with velocity and turbulence quantities fields from LES. These values are interpolated from the particle position using the cell points. The algebraic RANS turbulence model, Eq.(7), provides the turbulence quantities required to move the particles, using the LES velocity fluctuations.

The transport of the particle in composition space is modelled by reactions and micromixing. The reactions are simulated with finite-rate chemistry and a GPU-based explicit ODE solver has been used within the Lagrangian solver [22]. Since a ODE system has to be solved for each particle, the chemistry solution represents the most computational expensive part of the algorithm. However, the GPU architecture allows parallel optimization and reduction in computational time.

According to the MCL micromixing model, the mixing particles are randomly selected in a cell and the composition is modified towards their average values, following the Eq.(5). The mixing time scale is given by the inverse of Eq.(9). A dedicated algorithm controls that the particle number in each cell is kept between 20 and 25. If the particle number exceeds this value, particles with small weight are clustered; if the number is smaller, the heaviest particles are split in two with equal weight.

Simulation Setup

To evaluate the efficiency and accuracy of the hybrid method, simulations have been performed for the Sandia-D flame configuration [12]. The inner jet is a methane-air mixture in volume ratio $1:3$ at temperature of 294 K, corresponding to mixture fraction $f = 1$. The nozzle has an inner diameter of $D = 7.2\,mm$. The flame is stabilized using a pilot jet consisting of a burnt lean mixture methane/air at equivalence ratio of 0.77 and temperature of $1880\,K$. The coflow is air stream at 291 K. The flame D has a Reynolds number of 22400 and shows a small degree of local extinction [12].

The LES simulation is performed on a cylindrical domain of $60D * 5D$, discretized in 1 million of grid cells. The RANS simulation is performed on the same domain using a coarser grid (128000 cells),obtained reducing the resolution in circumferential direction. This allows a reduction of the computation requirements without decreasing the accuracy. This is valid limited to slow variations of the species mass fractions in space, like in the examined case. The RANS turbulent Schmidt number is set to $\sigma_t = 0.8$. The chemical reactions are simulated with finite-rate chemistry model using the Smooke kinetics mechanism, which includes 16 species and a 46 steps reaction [23]. The GPU-ODE integration is performed on a double precision GPU card NVIDIA Tesla K40.

Results and Discussion

The validation of the algebraic turbulence model has been firstly carried out. To check the consistency of the model, an Eulerian RANS simulation using the classical $k-\epsilon$ turbulence model has been performed on the same RANS-PDF grid. The results of the LES resolved turbulent kinetic energy $k_{t,res}$ are compared with the RANS turbulent kinetic energy k and experimental data on the axis and at three radial positions, $x/D = 7.5$, 15 and 30, in Fig. 1.

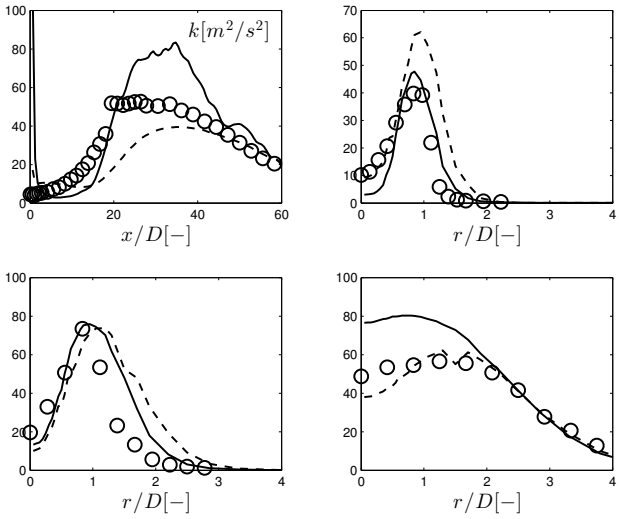

Figure 1: Comparison of the resolved turbulent kinetics energy $k_{t,res}$ extracted from LES (solid line) and obtained with the $k-\epsilon$ model (dashed line) with experimental data (circle) on the axis (top-left) and at radial position $x/d = 7.5$ (top-right) and $x/d = 15$ and 30 (bottom), respectively.

Fig. 1 shows an overprediction of the kinetic energy $k_{t,res}$ between downstream locations 20 and $45D$ on the axis. However, the radial profiles shows that the overprediction is limited to the inner mixing layer, $r/D < 2$. These results represent a preliminary work. Therefore, an improvement of the inflow boundary conditions of the LES simulation is required to reproduce a better LES flowfield. The profiles of the turbulent dynamic viscosity μ_t and dissipation ϵ obtained with the algebraic model and with the classical $k-\epsilon$ model on the axis and at radial positions are shown in Figs. 2 and 3. The radial profiles show

an underestimation of the turbulent viscosity and consequently overestimation of the dissipation. However, these results show that, for this particular geometry, the algebraic model provides reasonable RANS turbulent quantities and that, in principle, it is possible, using the more accurate LES solution, to extract the turbulence quantities for a RANS-PDF simulation.

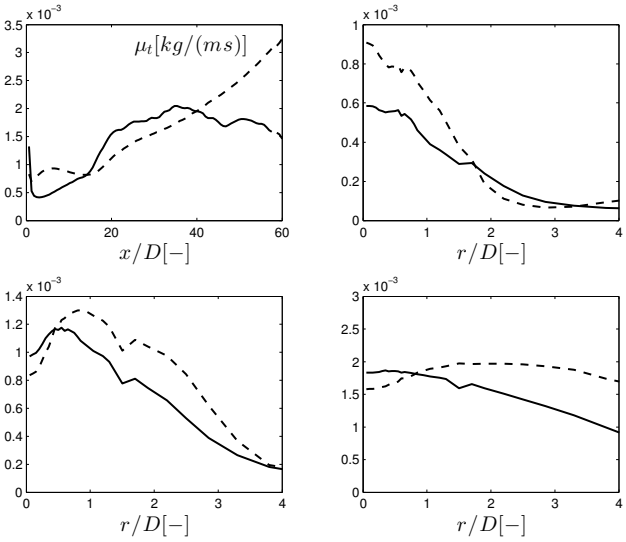

Figure 2: Comparison of the turbulent viscosity profiles on the axis (top-left) and at radial position $x/d = 7.5$ (top-right) and $x/d = 15$ and 30 (bottom), respectively. (solid line: algebraic model; dashed line: $k - \epsilon$ model)

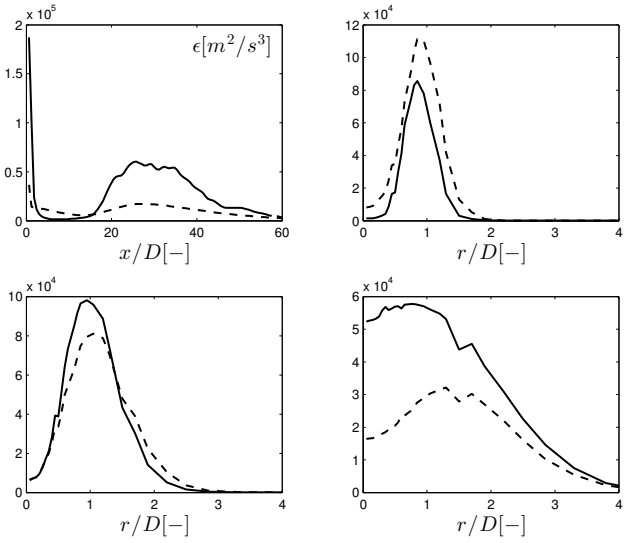

Figure 3: Comparison of the turbulent dissipation profiles on the axis (top-left) and at radial position $x/d = 7.5$ (top-right) and $x/d = 15$ and 30 (bottom), respectively. (solid line: algebraic model; dashed line: $k - \epsilon$ model)

Figure 4 shows preliminary results of the mixture fraction and temperature profiles obtained with the RANS-PDF solver, on the axis and at axial position $x/D = 7.5$. The simulation is still not completely converged, but from a qualitative analysis of the results, it may be seen the hybrid method is able to capture the turbulent reacting flame.

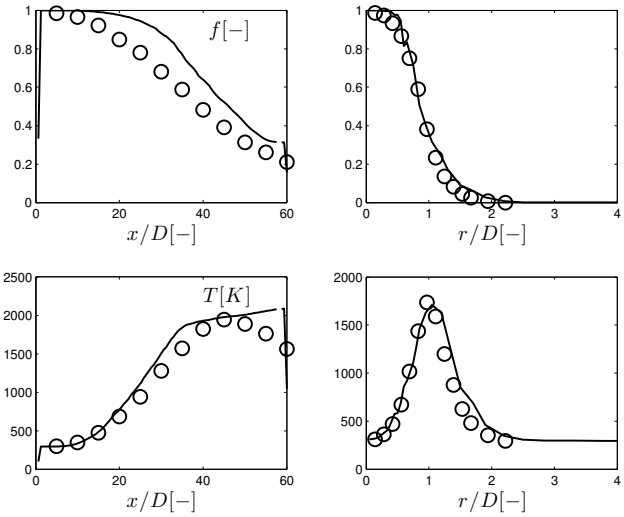

Figure 4: Comparison of the average mixture fraction on the axis and at radial position $x/d = 7.5$ (top) and of the average temperature on the axis and at radial position $x/d = 7.5$ (bottom) with the experimental data. (circle: Exp. data; solid line: RANS-PDF simulation)

Conclusions and Future works

A new implementation of the hybrid LES-RANS PDF model within OpenFOAM has been presented in this work. The full consistency of the hybrid method has been studied. Mean velocity and turbulent quantities, as the turbulent viscosity and frequency, are required in the RANS-PDF solver and provided by the LES solver. A model is needed to share these variables from LES to RANS context. A simple algebraic turbulence model has been used here as preliminary examination. In spite of its simplicity, the results show that the consistency has been achieved using this turbulence model, which is, however, limited to the jet flow configuration. Moreover, the new implementation of the whole algorithm within OpenFOAM coupled with the GPU-based ODE chemistry solver has been tested. The preliminary results of the RANS-PDF mixture fraction and temperature show that the hybrid method is able to simulate the reacting flame.

Further developments require a generalized turbulence model. Other methods will be implemented and compared with the algebraic model. The hypothesis of turbulence in local equilibrium, in which the dissipation ϵ is equal to the turbulence generation, will be tested. A second option will be to use the hypothesis of constant dissipation ϵ in the LES subgrid, according to Kolmogorov's turbulence

cascade theory, also for the RANS simulation.
Additional investigations will be directed to analyse the potential of the hybrid methods in terms of accuracy of the solution and computational efficiency.

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