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A consistent hybrid LES-RANS PDF method for non-premixed flames

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Abstract

The computational demanding LES methods have widely demonstrated their reliability in the description of large scale unsteady phenomena in turbulent reactive flows. RANS Transported Probability Density Function (TPDF) methods treat the nonlinear chemical reactions in closed form on relatively coarse grids and using a smaller number of stochastic particles. Combining the two approaches, a hybrid LES-RANS PDF method to predict non-premixed turbulent flames is presented. In this method a LES, based on Smagorinsky's model and steady flamelet, is performed; subsequently, the calculated flow-field is used to drive the RANS-TPDF equation, which is closed at the joint scalar level and based on a Lagrangian Monte Carlo scheme. The required velocity and turbulent quantities for RANS simulation are estimated from the resolved LES and an algebraic model based on dimensional analysis and the mixing length hypothesis. The results of the velocity, turbulent kinetic energy and mixture fraction show that the consistency of the method is achieved.

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Keywords: Hybrid model; Consistency LES-RANS; Turbulence; PDF methods; non-premixed combustion

1. Introduction

In the last decades LES has been used for simulations of complex turbulent flows. This method is able to resolve large scale flow structures, but finds its limitations in the high computational requirements for fine mesh and time resolutions [1]. On the other hand, 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 over-prediction 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. Past works have demonstrated the ability of PDF models to simulate non-premixed flames [5,6].
To overcome the limitations of each method and to obtain reliable results with high computational efficiency, different hybrid methods are proposed.

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Early hybrid LES/RANS models are based on the concept to perform a LES only in regions where it is needed and RANS simulation everywhere else, where this is enough accurate and reliable [2]. This requires that the two turbulent models match at the interface between the two zones, to guarantee a continuous velocity field. In turbulent reactive flows, different approaches, which include PDF as subgrid LES model, have been recently proposed. A large number of particles has to be used in each cell to build a representative PDF, requiring high computational effort [7]. An alternative "sparse" Lagrangian FDF method has been formulated in [8,9]. 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 of the hybrid LES/RANS-Lagrangian PDF method, firstly described in [1], are presented. The accurate LES flow field representation is applied along with the joint composition RANS-PDF to simulate turbulent non-premixed flows. In this way the quality and cost of the model are optimized. However, the LES/RANS coupling creates a consistency issue for the intrinsic theoretical differences of the two models, dealing with the sharing of some LES quantities into the RANS context. Mean velocity and turbulence quantities are required to close RANS joint composition-PDF equation, where Lagrangian particles move in a much coarser grid. We propose a consistent method to transfer this information from LES to RANS, based on the ensemble average LES quantities and a algebraic turbulence model.

2. Transport equation of the conditional composition PDF and hybrid LES RANS-TPDF model

In turbulent diffusion flames, reactive scalars Y_i depend on mixture fraction f, which describes the mixing of fuel and oxidizer [10]. 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 [11],

$$\frac{\partial}{\partial t}\left(\bar{\rho}\,\widetilde{P_f}\right)+\nabla\left(\bar{\rho}\tilde{v}\,\widetilde{P_f}\right)+\frac{\partial}{\partial\psi_i}\left(\bar{\rho}\langle W_i|\psi\ =f\rangle\widetilde{P_f}\right)=-\frac{\partial^2}{\partial\psi_i\partial\psi_j}\left(\bar{\rho}\langle \mathrm{D}\left(\nabla Y_i\nabla Y_j\right)|\psi=f\rangle\widetilde{P_f}\right)\ -\nabla\left(\bar{\rho}\langle v''|\psi=f\rangle\widetilde{P_f}\right) \qquad (1)$$

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 MC-method, used by [4], can be also used to solve the conditional PDF. In this work we follow the approach proposed in [11]: the MC-method is used to obtain the unconditional joint PDF. We assume to know for a specific fluid problem the stationary joint PDF of the reacting scalars, P(**Y**), which consists of mixture fraction, species mass fraction and enthalpy. The conditional PDF can be bijectively obtained using Bayes' theorem [12]. In this way it is possible to determine the unconditional PDF using the standard 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 $P^*(\Phi) = P_{f,MC}(\Phi)P_{LES}(f)$. This approach minimizes the cost decomposing the PDF transport equation in a part describing the transport of mixture fraction, extracted from LES, and another part representing the transport of species PDF conditioned on mixture fraction, obtained with the RANS-TPDF simulation.
The solution algorithm is divided in two parts: firstly an Eulerian LES, based on the incompressible Favre filtered transport equations for mass, momentum and mixture fraction, is performed; subsequently, a Lagrangian RANS composition-PDF is carried out. In RANS-TPDF, the particle evolution is governed by the stochastic differential equation [4]

$$dx_i^{(p)}=\left(\widetilde{u_i}+\frac{1}{\bar{\rho}}\frac{\partial}{\partial x_i}\left(\rho D_{eff}\right)\right)dt+\sqrt{2D_{eff}}dW_i \qquad (2)$$

where $x_i^{(p)}$e is the position of the stochastic particle p in physical space, $\widetilde{u_i}$ 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. (2) the required mean velocity, density and turbulent diffusivity quantities create a consistent issue. The procedure employed to share the LES quantities into the RANS context is presented in the next section. The density, obtained from the particles properties, is currently not fed back to the LES simulation.

3. Consistency of the hybrid method

The turbulence LES and RANS approaches work on different scales. In order to ensure consistency in the hybrid method, mean velocity field and turbulence quantities, required by Lagrangian RANS simulation, need to be evaluated from the averaged LES solution. Firstly the ensemble average LES flow field is generated. A large number of samples is 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 [13], $\langle\tilde{u}_i\rangle = \frac{\sum_{r=1}^{N_S} \widetilde{u_i^r}}{N_S}$, $\langle\tilde{u}''^2\rangle = \frac{\sum_{r=1}^{N_S} \widetilde{u_i^r}}{N_S} - \langle\tilde{u}_i\rangle^2$, the ensemble averaged LES velocity field and squared velocity resolved fluctuations, respectively, which correspond to RANS quantities.
The next task of the consistency deals with the turbulent variables. In this work a simple algebraic model is proposed to get the RANS turbulent viscosity, according to the dimensional analysis: $\upsilon_{t,RANS} = C_k l_{mix}\sqrt{k_{t,res}}$, where C_k is a new model constant ($C_k = 0.3$is used here), $k_{t,res} = \frac{1}{2}\sum_i\langle\tilde{u}''^2\rangle$) the LES resolved turbulent kinetic energy and l_{mix} the turbulent length scale. The turbulent length scale is estimated as a mixing length [14], proportional to the width of the shear layer $l_{mix} = \frac{1}{5}(x + \frac{5}{2}D)$:, where α, x, and D are the mixing-length coefficient, characteristic of the flow configuration (α=0.08 for round jet), the axial distance from the nozzle and the nozzle diameter, respectively.

4. Numerical Setup

To check the consistency of the hybrid method, a simulation is carried out with the Sandia-D flame [15]. The LES simulation is performed on a cylindrical grid consisting of 1025x35x60 nodes in axial, circumferential and radial directions respectively, mapping a geometry of 70Dx30D. The code used is *flowsi*, described in detail in [16, 17]. The sub-grid scale closure is achieved by using the dynamic Germano model and flamelet model. For the RANS-TPDF a second order Lagrangian particle transport algorithm is used on a 2−D grid with 205x60 cells [1]. The RANS turbulent Schmidt number is set to σ_t=0.85. For details of the simulation, please see [1].

5. Results and Discussion

Fig. 1 shows the averaged LES axial velocity $\langle\tilde{u}_i\rangle$ the resolved turbulent kinetic energy $k_{t,res}$ and the mixture fraction *f* along the axis, as well as the radial distribution of these variables at two axial position, *x/D=15* and *30*. In the first plot the axial development of the mean axial velocity, obtained by averaging LES samples, is slightly over-predicted for *x/D>10*. In the second plot the axial distribution of the LES resolved turbulent kinetic energy shows a peak at *x/D≈10*, relating to an over-prediction of the average velocity fluctuations. This seems to be due the difficulty of the LES code to resolve the thin mixing layer strictly downstream of the nozzle, as reported in [17]. Results of the mixture fraction are used to analyse the proposed algebraic turbulence model. The axial distribution of *f*, obtained performing the hybrid LES/RANS simulation, is shown in the third plot. A slight overprediction can be observed downstream *x/D=40*, but satisfactory agreement in the lower part of the flame. The discrepancy between calculated and experimental *f* is probably due to an underestimation of the turbulent viscosity, which produces less turbulent mixing of the particles. Radial profiles of $\langle\tilde{u}_i\rangle$ and $k_{t,res}$ indicate that the width of the flame is captured. At both axial positions*, x/D=15,30* the velocity profiles are well predicted, and only at *x/D=30* slightly overestimated in the inner mixing layer, *r/D<1*, as well the $k_{t,res}$. Moreover, the decay of the turbulent kinetic energy is overestimated at *x/D=30*. Accurate predictions of the mean radial mixture fraction at both axial positions can be observed in the last plot. The well reproduced results indicate that, with the ensemble average method applied to LES simulation and the simple turbulent model, a consistent coupling LES/RANS can be achieved for this flame configuration.

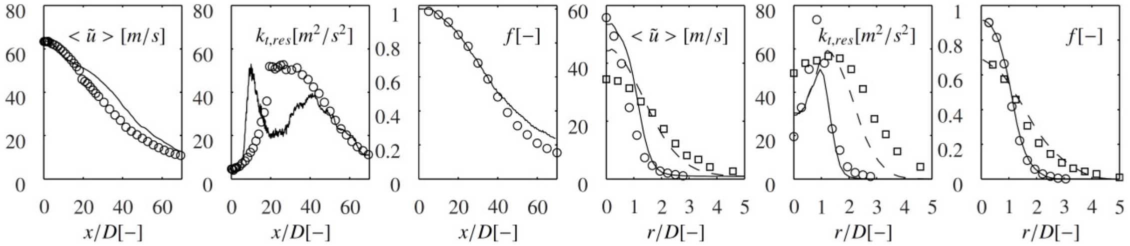

Figure 1. From left: Axial distribution of the mean axial velocity, resolved kinetic energy and mixture fraction (circle: Exp. data; solid line: LES/RANS); radial distribution of mean axial velocity, resolved turbulent kinetic energy and mixture fraction at *x/D=15* (circle: Exp. data; solid line: LES/RANS) and *x/D=30* (square: Exp. data; dashed line: LES/RANS).

6. Conclusions

A hybrid LES/RANS-PDF method has been introduced with a focus on the consistency between LES and RANS. The hybrid model allows to perform a LES with a simple chemistry model and then to improve the accuracy of the scalar prediction with the RANS Lagrangian PDF. The LES ensemble average solution is used to generate the required RANS mean quantities. The simple algebraic turbulence model is applied to obtain the turbulence viscosity. The proposed method shows good results on the mean mixture fraction prediction. The algebraic turbulence model is quite promising; however, it is limited to the jet flow configuration. Further developments require a generalized procedure to obtain Reynolds stresses and length scales consistent with the LES.

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