CONTRIBUTION TO THE VARIATIONAL CALCULUS OF THE HYBRID RANS/LES PITM METHOD FOR THE SIMULATION OF TURBULENT FLOWS

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Abstract

Non-zonal hybrid RANS/LES methods are of practical interest for engineering applications. Among these methods, the partially integrated transport modeling (PITM) that varies continuously form RANS to DNS depends on a control parameter linked to the grid step size initially developed in spectral space for homogeneous turbulence. We show that variational calculus formally recovers the spectral PITM model derivation and extend its field of application to the case of non-homogeneous flows.

1 Introduction

Among the hybrid RANS-LES methods that have been developed in the past twenty years (Chaouat, 2017; Schiestel and Chaouat, 2022), the partially integrated transport modeling (PITM) method developed by Schiestel and Dejoan (2005) in the framework of eddy viscosity models (EVM) and Chaouat and Schiestel (2005) in second moment closure (SMC) allows us to transpose any RANS model into its hybrid LES counterpart with seamless coupling between the RANS and LES prevailing regions. Depending on the closure of the equations, the two-equation model accounting for the subfilter turbulent energy $k^{(s)}$ and its dissipation-rate $\epsilon^{(s)}$ in EVM is rather used for engineering applications because of its numerical robustness whereas the subfilter stress $\tau_{ij}^{(s)}$ and $\epsilon^{(s)}$ developed in the framework of second moment closure (SMC) (Schiestel, 2008) is more appropriate for academic flows with emphasis on fundamental aspects and requires an appropriate numerical procedure to be applied (Chaouat 2011). These EVM and SMC models relie on the control function appearing in the dissipation-rate transport equation $\epsilon^{(s)}$ that is represented as an adjustable varying parameter in the source/sink term such that

$$C_{\epsilon_2}^{(s)} = C_{\epsilon_1}^{(s)} + R(r)\left(C_{\epsilon_2} - C_{\epsilon_1}\right) \tag{1}$$

where C_{ϵ_1} and C_{ϵ_2} are the constant coefficients used in the RANS dissipation-rate equation and $R(r)$, a function of $r = k^{(s)}/k$ defined as the ratio of the modeled turbulence subfilter energy to the total energy. Considering that the $R(r)$ function deserves a major importance in PITM simulations, we will show that the linear equation $R(r) = r$ obtained previously for homogeneous flows in the spectral space (Chaouat and Schiestel, 2005, 2007) can be formally recovered in a mathematical sense from variational calculus in a general case of non-homogeneous flows. An extension to the transport equations for the passive scalar including the half-scalar variance $k_\theta^{(s)}$ and its dissipation rate $\epsilon_\theta^{(s)}$ will be also undertaken and we will show that the linear equation $R_\theta(r_\theta) = r_\theta$ where $r_\theta = k_\theta^{(s)}/k_\theta$ is still verified. The variational calculus is also useful to link together different hybrid RANS/LES models (Friess and Davidson 2020).

2 Variational analysis

Viscous incompressible flow is considered here. In RANS methodology, each variable ϕ is then decomposed into a statistical mean part $\langle\phi\rangle$ and a fluctuating part ϕ' such that $\phi = \langle\phi\rangle + \phi'$ whereas in large eddy simulations, the variable ϕ is decomposed into a large scale (or resolved part) $\bar{\phi}$ and a subfilter-scale fluctuating part $\phi^{>}$ or modeled part such that $\phi = \bar{\phi} + \phi^{>}$. The eddy viscosity PITM model consists in solving the instantaneous filtered equations including the momentum equation coupled with the $k^{(s)}$ and $\epsilon^{(s)}$ equations represented in a mathematical form by (Chaouat and Schiestel, 2021)

$$\begin{cases} \mathcal{K}(\bar{u_i}, k^{(s)}, \epsilon^{(s)}) = 0 \\ \mathcal{E}(\bar{u_i}, k^{(s)}, \epsilon^{(s)}, R) = 0 \end{cases} \tag{2}$$

where $\bar{u_i}$ is the filtered velocity, with appropriate boundary conditions and initial conditions. The parameters $k^{(s)}$, $\epsilon^{(s)}$, R are some functions of space x_i and time t, while $\mathcal{K}$ and $\mathcal{E}$ denote functionals. Supposing model self-consistency, the variational system

to solve, associated with (2) reads

$$\begin{cases} \boldsymbol{\delta}\mathcal{K} = \left(\dfrac{\boldsymbol{\partial}\mathcal{K}}{\boldsymbol{\partial} k_s}\right)\boldsymbol{\delta} k^{(s)} + \left(\dfrac{\boldsymbol{\partial}\mathcal{K}}{\boldsymbol{\partial}\epsilon_s}\right)\boldsymbol{\delta}\epsilon^{(s)} = 0 \\ \quad \boldsymbol{\delta}\mathcal{E} = \left(\dfrac{\boldsymbol{\partial}\mathcal{E}}{\boldsymbol{\partial} k_s}\right)\boldsymbol{\delta} k^{(s)} + \left(\dfrac{\boldsymbol{\partial}\mathcal{E}}{\boldsymbol{\partial}\epsilon_s}\right)\boldsymbol{\delta}\epsilon^{(s)} \\ + \left(\dfrac{\boldsymbol{\partial}\mathcal{E}}{\boldsymbol{\partial} R}\right)\boldsymbol{\delta} R = 0 \end{cases} \tag{3}$$

The PITM method calculates the large scales and models the small scales. In practice, for steady flows in the mean, the system (3) can be considered in the statistical sense. Variations such as $\boldsymbol{\delta}k^{(s)}$ and $\boldsymbol{\delta}\epsilon^{(s)}$ are then random variables but not $\boldsymbol{\delta}R$ which is a numerical coefficient of the model itself.

General derivation for the dynamic variations in the $k^{(s)} - \epsilon^{(s)}$ model

The $k^{(s)}$-$\epsilon^{(s)}$ EVM based on the transport equations of the subfilter energy and its dissipation-rate is considered here but the following development prevails also for the $\tau_{ij}^{(s)} - \epsilon^{(s)}$ model. The transport equation for the subfilter energy reads

$$\frac{\mathcal{D}k^{(s)}}{\mathcal{D}t} = P_k^{(s)} - \epsilon^{(s)} + J_k^{(s)} + d_k^{(s)} \tag{4}$$

where the subfilter production is defined as

$$P_k^{(s)} = -\tau_{ij}^{(s)}\frac{\partial \overline{u}_i}{\partial x_j} \tag{5}$$

the turbulent diffusion term is modeled as

$$J_k^{(s)} = \frac{\partial}{\partial x_j}\left(C_k \frac{{k^{(s)}}^2}{\epsilon^{(s)}}\frac{\partial k^{(s)}}{\partial x_j}\right) \tag{6}$$

where C_k is a constant coefficient, and the molecular diffusion reads

$$d_k^{(s)} = \frac{\partial}{\partial x_j}\left(\nu\frac{\partial k^{(s)}}{\partial x_j}\right) \tag{7}$$

The transport equation for the subfilter dissipation-rate reads

$$\frac{\mathcal{D}\epsilon^{(s)}}{\mathcal{D}t} = C_{\epsilon_1}^{(s)}\frac{P_k^{(s)}\epsilon^{(s)}}{k^{(s)}} - C_{\epsilon_2}^{(s)}\frac{{\epsilon^{(s)}}^2}{k^{(s)}} + J_\epsilon^{(s)} + d_\epsilon^{(s)} \tag{8}$$

where the turbulent diffusion term is modeled as

$$J_\epsilon^{(s)} = \frac{\partial}{\partial x_j}\left(C_\epsilon \frac{{k^{(s)}}^2}{\epsilon^{(s)}}\frac{\partial \epsilon^{(s)}}{\partial x_j}\right) \tag{9}$$

where C_ϵ is a constant coefficient, and the molecular diffusion reads

$$d_\epsilon^{(s)} = \frac{\partial}{\partial x_j}\left(\nu\frac{\partial \epsilon^{(s)}}{\partial x_j}\right) \tag{10}$$

In Equations (4) and (8), $\mathcal{D}/\mathcal{D}t = \partial/\partial t + \bar{u}_j\partial/\partial x_j$ denotes the derivative along the filtered velocity field. In Equation (8), $C_{\epsilon_1}^{(s)} = C_{\epsilon_1}$ is a constant coefficient while $C_{\epsilon_2}^{(s)}$ given by Eq. (1) is a dynamic coefficient in the PITM method (Schiestel and Dejoan, 2005, Chaouat and Schiestel, 2005). The subfilter turbulent stress $\tau_{ij}^{(s)}$ is computed assuming the Boussinesq hypothesis where the turbulent eddy viscosity is given by

$$\nu_t^{(s)} = C_\nu \frac{{k^{(s)}}^2}{\epsilon^{(s)}} \tag{11}$$

C_ν is a constant coefficient. The changes in the solution occurring in a functional space are described by the functional variations (3) in the turbulent field. For flows close to equilibrium, it is reasonable to assume that the material derivatives of any subgrid variable $\phi^{(s)}$ along mean streamlines is negligible leading to

$$\frac{D\left\langle\phi^{(s)}\right\rangle}{Dt} = \frac{\partial\left\langle\phi^{(s)}\right\rangle}{\partial t} + \langle u_j\rangle\frac{\partial\left\langle\phi^{(s)}\right\rangle}{\partial x_j} = 0 \tag{12}$$

where $\phi = k^{(s)}$ or $\epsilon^{(s)}$, so that $D\left\langle k^{(s)}\right\rangle/Dt = 0$ and $D\left\langle\epsilon^{(s)}\right\rangle/Dt = 0$. Consequently, averaging Equations (4) and (8) leads to

$$\begin{aligned}\frac{D\left\langle k^{(s)}\right\rangle}{Dt} &= \left\langle P_k^{(s)}\right\rangle - \left\langle\epsilon^{(s)}\right\rangle + \left\langle J_k^{(s)}\right\rangle \\ &+ \left\langle j_k^{(r)}\right\rangle + \left\langle d_k^{(s)}\right\rangle\end{aligned} \tag{13}$$

and

$$\begin{aligned}\frac{D\left\langle\varepsilon^{(s)}\right\rangle}{Dt} &= C_{\epsilon_1}^{(s)}\frac{\left\langle P_k^{(s)}\right\rangle\left\langle\varepsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} - C_{\epsilon_2}^{(s)}\frac{\left\langle\varepsilon^{(s)}\right\rangle^2}{k^{(s)}} \\ &+ \left\langle J_\epsilon^{(s)}\right\rangle + \left\langle j_\epsilon^{(r)}\right\rangle + \left\langle d_\epsilon^{(s)}\right\rangle\end{aligned} \tag{14}$$

where

$$j_k^{(r)}\left(k^{(s)}\right) = -\frac{\partial}{\partial x_j}\left(u_j^{<}k^{(s)}\right) \tag{15}$$

and

$$j_\epsilon^{(r)}\left(\epsilon^{(s)}\right) = -\frac{\partial}{\partial x_j}\left(u_j^{<}\epsilon^{(s)}\right) \tag{16}$$

are the new additional terms arising from the statistical procedure assuming the physical hypothesis (12). In order to pursue the variational analysis, the exact resolved flux denoted $\left\langle j_\phi^{(r)}\right\rangle$ for both $\left\langle j_k^{(r)}\right\rangle$ or $\left\langle j_\epsilon^{(r)}\right\rangle$ are analytically modeled assuming a gradient diffusion law as

$$\left\langle J_\phi^{(r)}\left(\phi\right)\right\rangle = C_\phi\frac{\partial}{\partial x_j}\left[\frac{\left\langle k^{(r)}\right\rangle^2}{\left\langle\epsilon^{(s)}\right\rangle}\frac{\partial\langle\phi\rangle}{\partial x_j}\right] \tag{17}$$

At this step, it is of importance for the following to make clear the difference between the exact contribution $\left\langle j_\phi^{(r)}\right\rangle$ and its corresponding modeling $\left\langle J_\phi^{(r)}\right\rangle$. Using (17), the total diffusion term can be computed as

$$\begin{aligned}\left\langle J_\phi^{(s+r)}\right\rangle &= \left\langle J_\phi^{(s)} + J_\phi^{(r)}\right\rangle \\ &\approx C_\phi\frac{\partial}{\partial x_j}\left[\frac{\left\langle k^{(s+r)}\right\rangle^2}{\left\langle\epsilon^{(s)}\right\rangle}\frac{\partial\langle\phi\rangle}{\partial x_j}\right]\end{aligned} \tag{18}$$

Analytical solution for the $k^{(s)}-\epsilon^{(s)}$ model

Equilibrium in a statistical sense in Eqations (13) and (14) using (18) leads to the two balance equations

$$\left\langle P_k^{(s)}\right\rangle = \left\langle \epsilon^{(s)}\right\rangle - \left\langle J_k^{(s+r)}\right\rangle \tag{19}$$

and

$$C_{\epsilon_1}^{(s)}\frac{\left\langle P_k^{(s)}\right\rangle\left\langle \epsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} - C_{\epsilon_2}^{(s)}\frac{\left\langle \epsilon^{(s)}\right\rangle^2}{\left\langle k^{(s)}\right\rangle} = -\left\langle J_\epsilon^{(s+r)}\right\rangle \tag{20}$$

Combining Equations (1), (19), (20) provides the resulting equation to be solved

$$R(r)\frac{\Delta C_\epsilon}{\left\langle J_\epsilon^{(s+r)}\right\rangle}\frac{\left\langle \epsilon^{(s)}\right\rangle^2}{\left\langle k^{(s)}\right\rangle} = \left[1 - C_{\epsilon_1}\frac{\left\langle \epsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle}\frac{\left\langle J_k^{(s+r)}\right\rangle}{\left\langle J_\epsilon^{(s+r)}\right\rangle}\right] \tag{21}$$

where $\Delta C_\epsilon = C_{\epsilon_2} - C_{\epsilon_1}$ or

$$R(r)\Delta C_\epsilon\frac{\left\langle \epsilon^{(s)}\right\rangle^2}{\left\langle k^{(s)}\right\rangle} = E\left\langle J_\epsilon^{(s+r)}\left(\epsilon^{(s)}\right)\right\rangle, \tag{22}$$

where

$$E = 1 - C_{\epsilon_1}\frac{\left\langle \epsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle}\frac{\left\langle J_k^{(s+r)}\left(k^{(s)}\right)\right\rangle}{\left\langle J_\epsilon^{(s+r)}\left(\epsilon^{(s)}\right)\right\rangle}. \tag{23}$$

A long and tedious variational calculus of each function appearing in (22) finally yields the simple expression (Chaouat and Schiestel, 2023)

$$\frac{\boldsymbol{\delta} R(r)}{R(r)} = \frac{\boldsymbol{\delta}\left\langle k^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} - 2\frac{\boldsymbol{\delta}\left\langle \epsilon^{(s)}\right\rangle}{\left\langle \epsilon^{(s)}\right\rangle} \tag{24}$$

Keeping in mind that $\left\langle \epsilon^{(s)}\right\rangle$ is not affected by the cutoff wave number $\partial\epsilon^{(s)}/\partial\kappa_c = 0$ because it represents the flux of energy that is transferred from the large scales to the small scales (Chaouat and Schiestel, 2012), Equation (24) reduces to

$$\frac{\boldsymbol{\delta} R(r)}{R(r)} = \frac{\boldsymbol{\delta}\left\langle k^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} \tag{25}$$

and from path functional integration

$$\int_R^1 \frac{\boldsymbol{\delta} R}{R} = \int_{\left\langle k^{(s)}\right\rangle}^k \frac{\boldsymbol{\delta}\left\langle k^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} \tag{26}$$

leading to the expected result

$$R(r) = \frac{\left\langle k^{(s)}\right\rangle}{k} = r \tag{27}$$

as previously found in the PITM method considering the energy flux transfer in the spectral space (Chaouat and Schiestel, 2005, 2007, 2012). This result differs from what has been found by Heinz (2021,2022) who performed variational calculus yielding $R(r) = r^3$ essentially because the resolved diffusion terms (15) and (16) were not accounted for.

General derivation for the passive scalar variations in the $k_\theta^{(s)}$-$\epsilon_\theta^{(s)}$ model

The case of a passive scalar transport field is considered where $k_\theta^{(s)}$ and $\epsilon_\theta^{(s)}$ are the scalar variance and its dissipation rate. For EVM, the scalar flux transfer is computed as

$$\tau_{i\theta}^{(s)} = -C_{\tau_\theta}\frac{{k^{(s)}}^2}{\epsilon^{(s)}}\frac{\partial\bar{\theta}}{\partial x_i} \tag{28}$$

where C_{τ_θ} is a numerical coefficient. The transport equation for the subfilter half-scalar variance $k_\theta^{(s)}$ reads (Chaouat and Schiestel, 2021)

$$\frac{\mathcal{D}k_\theta^{(s)}}{\mathcal{D}t} = P_\theta^{(s)} - \epsilon_\theta^{(s)} + J_{k_\theta}^{(s)} + d_{k_\theta}^{(s)} \tag{29}$$

where the subfilter production $P_\theta^{(s)}$ is given by

$$P_\theta^{(s)} = -\tau_{j\theta}^{(s)}\frac{\partial\bar{\theta}}{\partial x_j} \tag{30}$$

The turbulent diffusion term $J_{k_\theta}^{(s)}$ is modeled using a simple gradient law hypothesis

$$J_{k_\theta}^{(s)} = \frac{\partial}{\partial x_j}\left(C_{k_\theta}\frac{{k^{(s)}}^2}{\epsilon^{(s)}}\frac{\partial k_\theta^{(s)}}{\partial x_j}\right) \tag{31}$$

where C_{k_θ} is a constant coefficient and the molecular diffusion reads

$$d_{k_\theta}^{(s)} = \frac{\partial}{\partial x_j}\left(\sigma\frac{\partial k_\theta^{(s)}}{\partial x_j}\right) \tag{32}$$

where $\sigma = \nu/P_r$ and P_r denotes the molecular Prandtl number. The transport equation for the subfilter dissipation-rate $\epsilon_\theta^{(s)}$ in its general formulation reads (Chaouat, 2021)

$$\frac{\mathcal{D}\epsilon_\theta^{(s)}}{\mathcal{D}t} = C_{\epsilon_{\theta\theta_1}}^{(s)}P_\theta^{(s)}\frac{\epsilon_\theta^{(s)}}{k_\theta^{(s)}} + C_{\epsilon_{\theta k_1}}^{(s)}P_k^{(s)}\frac{\epsilon_\theta^{(s)}}{k^{(s)}}$$
$$-C_{\epsilon_{\theta k_2}}^{(s)}\frac{\epsilon_\theta^{(s)}\epsilon^{(s)}}{k^{(s)}} - C_{\epsilon_{\theta\theta_2}}^{(s)}\frac{{\epsilon_\theta^{(s)}}^2}{k_\theta^{(s)}} + J_{\epsilon_\theta}^{(s)} + d_{\epsilon_\theta}^{(s)} \tag{33}$$

where the coefficients appearing in Eq. (33) are given by Chaouat and Schiestel (2021) $C_{\epsilon_{\theta\theta_1}}^{(s)} = C_{\epsilon_{\theta\theta_1}} = 1$, $C_{\epsilon_{\theta k_1}}^{(s)} = C_{\epsilon_{\theta k_1}} = 1/2$, $C_{\epsilon_{\theta k_2}}^{(s)} = C_{\epsilon_{\theta k_2}} = 1/2$. and $C_{\epsilon_{\theta\theta_2}}^{(s)}$ is computed as

$$C_{\epsilon_{\theta\theta_2}}^{(s)} = C_{\epsilon_{\theta\theta_1}} + R_\theta(r_\theta)\left(C_{\epsilon_{\theta\theta_2}} - C_{\epsilon_{\theta\theta_1}}\right) \tag{34}$$

where R_θ is a function of $r_\theta = k_\theta^{(s)}/k_\theta$. The turbulent diffusion term $J_{\epsilon_\theta}^{(s)}$ is modeled using a simple gradient law hypothesis

$$J_{\epsilon_\theta}^{(s)} = \frac{\partial}{\partial x_j}\left(C_{\epsilon_\theta}\frac{{k^{(s)}}^2}{\epsilon^{(s)}}\frac{\partial\epsilon_\theta^{(s)}}{\partial x_j}\right) \tag{35}$$

where C_{ϵ_θ} is a constant coefficient. The molecular diffusion reads

$$d_{\epsilon_\theta}^{(s)} = \frac{\partial}{\partial x_j}\left(\sigma \frac{\partial \epsilon_\theta^{(s)}}{\partial x_j}\right) \tag{36}$$

The equations (29) and (33) can be rewritten as

$$\frac{Dk_\theta^{(s)}}{Dt} = P_\theta^{(s)} - \epsilon_\theta^{(s)} + J_{k_\theta}^{(s)} + j_{k_\theta}^{(r)} + d_{k_\theta}^{(s)} \tag{37}$$

$$\begin{aligned}\frac{D\epsilon_\theta^{(s)}}{Dt} &= C_{\epsilon_{\theta\theta_1}}^{(s)} P_\theta^{(s)} \frac{\epsilon_\theta^{(s)}}{k_\theta^{(s)}} + C_{\epsilon_{\theta k_1}}^{(s)} P_k^{(s)} \frac{\epsilon_\theta^{(s)}}{k^{(s)}} \\ &- C_{\epsilon_{\theta k_2}}^{(s)} \frac{\epsilon_\theta^{(s)} \epsilon^{(s)}}{k^{(s)}} - C_{\epsilon_{\theta\theta_2}}^{(s)} \frac{{\epsilon_\theta^{(s)}}^2}{k_\theta^{(s)}} + J_{\epsilon_\theta}^{(s)} + j_{\epsilon_\theta}^{(r)} \\ &+ d_{\epsilon_\theta}^{(s)}\end{aligned} \tag{38}$$

where

$$j_\phi^{(r)}(\phi_\theta) = -\frac{\partial}{\partial x_j}\left(u_j^< \phi_\theta\right) \tag{39}$$

for $\phi_\theta = k_\theta^{(s)}$ or $\phi_\theta = \epsilon_\theta^{(s)}$. We take then the averaging of Equations (37) and (38). The exact diffusion term $\left\langle j_\phi^{(r)}(\phi_\theta)\right\rangle$ can be modeled by

$$\left\langle J_\phi^{(r)}\right\rangle = C_{\phi\theta}\frac{\partial}{\partial x_j}\left[\frac{\left\langle k^{(r)}\right\rangle^2}{\left\langle \epsilon^{(s)}\right\rangle}\frac{\partial\langle\phi_\theta\rangle}{\partial x_j}\right] \tag{40}$$

so that in a first approximation, the total turbulent diffusion terms $J_\phi^{(s+r)}$ reads

$$\left\langle J_\phi^{(s+r)}\right\rangle = C_{\phi\theta}\frac{\partial}{\partial x_j}\left[\frac{\left\langle k^{(s+r)}\right\rangle^2}{\left\langle \epsilon^{(s)}\right\rangle}\frac{\partial\langle\phi_\theta\rangle}{\partial x_j}\right] \tag{41}$$

Using the hypothesis of equilibrium along mean streamlines implying that $D/Dt = 0$, considering that the molecular diffusion terms are small, it is then possible to obtain the equations for the variance $k_\theta^{(s)}$ and its dissipation-rate $\epsilon_\theta^{(s)}$ that must be solved.

Analytical solution for the $k_\theta^{(s)}$-$\epsilon_\theta^{(s)}$ model

This mathematical development leads to the two balance equations

$$\left\langle P_\theta^{(s)}\right\rangle - \left\langle \epsilon_\theta^{(s)}\right\rangle + \left\langle J_{k_\theta}^{(s+r)}\right\rangle = 0 \tag{42}$$

and

$$\begin{aligned}&C_{\epsilon_{\theta\theta_1}}^{(s)}\left\langle P_\theta^{(s)}\right\rangle \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle}{\left\langle k_\theta^{(s)}\right\rangle} + C_{\epsilon_{\theta k_1}}^{(s)}\left\langle P_k^{(s)}\right\rangle \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} \\ &- C_{\epsilon_{\theta k_2}}^{(s)} \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle\left\langle \epsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} - C_{\epsilon_{\theta\theta_2}}^{(s)} \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle^2}{\left\langle k_\theta^{(s)}\right\rangle} + \left\langle J_{\epsilon_\theta}^{(s+r)}\right\rangle \\ &= 0\end{aligned} \tag{43}$$

Substituting the expression of the production terms $P_k^{(s)}$ and $P_\theta^{(s)}$ given by (19) and (42), respectively, into (43) and using (34) yields

$$\begin{aligned}&\Delta C_{\epsilon_{\theta k}} \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle\left\langle \epsilon^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} + R_\theta(r_\theta)\Delta C_{\epsilon_{\theta\theta}} \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle^2}{\left\langle k_\theta^{(s)}\right\rangle} \\ &= \left\langle J_{\epsilon_\theta}^{(s+r)}\right\rangle - C_{\epsilon_{\theta\theta_1}}\left\langle J_{k_\theta}^{(s+r)}\right\rangle \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle} \\ &- C_{\epsilon_{\theta k_1}}\left\langle J_k^{(s+r)}\right\rangle \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle}{\left\langle k^{(s)}\right\rangle}.\end{aligned} \tag{44}$$

where

$$\Delta C_{\epsilon_{\theta\theta}} = C_{\epsilon_{\theta\theta_2}} - C_{\epsilon_{\theta\theta_1}} \tag{45}$$

and

$$\Delta C_{\epsilon_{\theta k}} = C_{\epsilon_{\theta k_2}} - C_{\epsilon_{\theta k_1}} \tag{46}$$

or equivalently, the resulting equation is

$$R_\theta(r_\theta)\Delta C_{\epsilon_{\theta\theta}} \frac{\left\langle \epsilon_\theta^{(s)}\right\rangle^2}{\left\langle k_\theta^{(s)}\right\rangle} = \left\langle J_{\epsilon_\theta}^{(s+r)}\right\rangle F \tag{47}$$

where the function F is given by

$$F = 1 - \frac{A\left\langle \epsilon_\theta^{(s)}\right\rangle}{\left\langle J_{\epsilon_\theta}^{(s+r)}\right\rangle} \tag{48}$$

with

$$A = C_{\epsilon_{\theta\theta_1}} \frac{\left\langle J_{k_\theta}^{(s+r)}\right\rangle}{\left\langle k_\theta^{(s)}\right\rangle} - C_{\epsilon_{\theta k_1}} \frac{\left\langle J_k^{(s+r)}\right\rangle}{\left\langle k^{(s)}\right\rangle} \tag{49}$$

Considering that $\epsilon_\theta^{(s)}$ remains unaffected by the cut-off wave number location κ_c of the grid, i.e., $\partial\epsilon_\theta^{(s)}/\partial\kappa_c = 0$, the variational calculus of Equation (47) finally yields the simple expression (Chaouat and Schiestel, 2023)

$$\frac{\boldsymbol{\delta} R_\theta(r_\theta)}{R_\theta(r_\theta)} = \frac{\boldsymbol{\delta}\left\langle k_\theta^{(s)}\right\rangle}{\left\langle k_\theta^{(s)}\right\rangle} \tag{50}$$

and from path integration

$$\int_{R_\theta}^{1} \frac{\boldsymbol{\delta} R_\theta}{R_\theta} = \int_{\left\langle k_\theta^{(s)}\right\rangle}^{k_\theta} \frac{\boldsymbol{\delta}\left\langle k_\theta^{(s)}\right\rangle}{\left\langle k_\theta^{(s)}\right\rangle} \tag{51}$$

leading to

$$R_\theta(r_\theta) = \frac{\left\langle k_\theta^{(s)}\right\rangle}{k_\theta} = r_\theta \tag{52}$$

As a result of interest, Equation (52) is the same as the one found in the spectral space by considering the

different turbulent processes (Chaouat and Schiestel, 2021).

3 Numerical results

The well known fully developed turbulent channel flow is performed for illustrating the results of the variational calculus. The dimensions of the channel in the streamwise, spanwise and normal directions along the x_1, x_2, x_3 axes are $L_1 = 6.4\delta$, $L_2 = 3.2\delta$ and $L_3 = 2\delta$. The simulation is performed on a medium grid with resolution $84 \times 42 \times 256$ in the (x_1, x_2, x_3) directions. The grid in the normal direction to the wall is here refined not for the simulation itself but for accurately computing the exact resolved diffusion terms of the transport equations $k^{(s)}$-$\epsilon^{(s)}$ that will be compared with their corresponding modeling. The friction Reynolds number is $R_\tau = 395$ based on the friction velocity and the half channel width. The numerical code is based on an accurate finite volume technique (Chaouat, 2011). The $\tau_{ij}^{(s)} - \epsilon^{(s)}$ model is applied here because it reproduces fairly well the turbulence anisotropy (Chaouat and Schiestel, 2005, 2012). As usually, the results are presented in dimensionless form using the dynamical viscosity ν, the friction velocity u_τ. The profiles of the streamwise turbulence

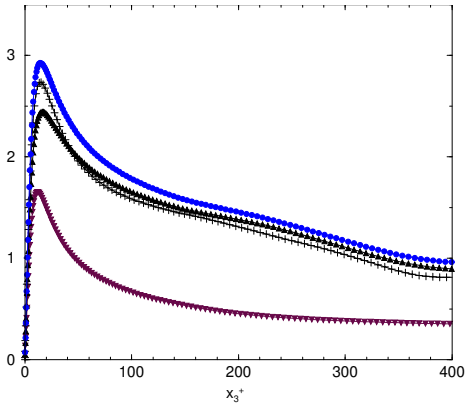

Figure 1: Streamwise turbulence intensity versus the wall distance. Subfilter scales $\left\langle \tau_{11}^{(s)+} \right\rangle^{1/2}$: ▼; Resolved scales $\left\langle \tau_{11}^{(r)+} \right\rangle^{1/2}$: ▲; Total scales $\left\langle \tau_{11}^{(s+r)+} \right\rangle^{1/2}$: ●; DNS $R_\tau = 395$ (Chaouat 2023) : +++.

intensities including the subfilter, resolved and total scales is presented in Figure 1 as a preliminary check. With the present grid refinement, the PITM model runs more or less in almost RANS mode in the near wall region and in LES mode when moving away from the wall. A good agreement is obtained with the DNS data. Figure 2 shows the profile of the exact resolved diffusion term $\left\langle j_k^{(r)} \right\rangle$ where $j_k^{(r)}$ is given by Eq. (15) and its modeled counterpart $\left\langle J_k^{(r)} \right\rangle$ in the framework

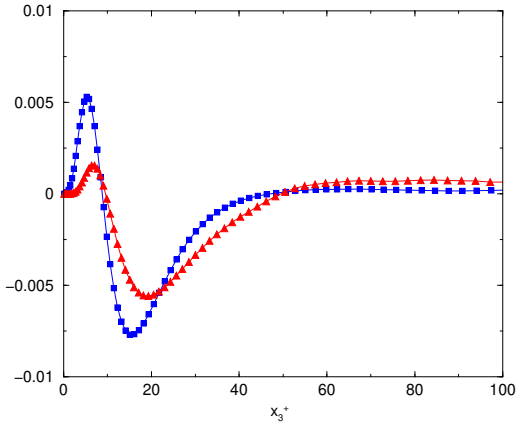

Figure 2: Diffusion of the resolved turbulent energy versus the wall unit distance. Simulation ■: $\left\langle j_k^{(r)+} \right\rangle$; Modeling ▲ : $\left\langle J_k^{(r)+} \right\rangle$.

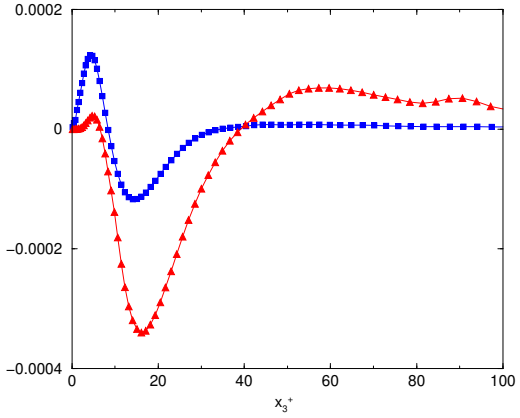

Figure 3: Diffusion of the resolved dissipation-rate versus the wall unit distance. Simulation ■: $\left\langle j_\epsilon^{(r)+} \right\rangle$; Modeling ▲ : $\left\langle J_\epsilon^{(r)+} \right\rangle$.

of SMC that reads

$$\left\langle J_k^{(r)} \right\rangle = C_k \frac{\partial}{\partial x_3} \left(\frac{\left\langle k^{(r)} \right\rangle}{\left\langle \epsilon^{(s)} \right\rangle} \left\langle \tau_{33}^{(r)} \right\rangle \frac{\partial \left\langle k^{(s)} \right\rangle}{\partial x_3} \right) \quad (53)$$

where $C_k = 0.22$, versus the wall distance of the channel in dimensionless wall unit. The modeled and resolved turbulent diffusion terms display the same regular evolution in the channel cross section although the modeled contribution is somewhat under-predicted. This should be attributed to the modeling (Chaouat, 2023). However, the important point to see is that the resolved contribution is not reduced to zero and must be therefore accounted for in the variational calculus as it has been made. Figure 3 shows the profile of the exact resolved diffusion term $\left\langle j_\epsilon^{(r)} \right\rangle$ where $j_\epsilon^{(r)}$ is given by Eq. (16) and its modeled counterpart $\left\langle J_\epsilon^{(r)} \right\rangle$

in the framework of SMC given by

$$\left\langle J_{\epsilon}^{(r)} \right\rangle = C_{\epsilon} \frac{\partial}{\partial x_3} \left(\frac{\left\langle k^{(r)} \right\rangle}{\left\langle \epsilon^{(s)} \right\rangle} \left\langle \tau_{33}^{(r)} \right\rangle \frac{\partial \left\langle \epsilon^{(s)} \right\rangle}{\partial x_3} \right) \quad (54)$$

where $C_{\epsilon} = 0.18$, versus the wall distance across the channel. The modeled and resolved turbulent diffusion terms exhibit roughly the same evolution in the channel cross section, even if some discrepancies in the order of magnitude are visible. This is probably due to the gradient law hypothesis that is not always closely verified. Once again, the significant achievement in this result is to emphasize that the resolved contribution cannot be considered as negligible. To

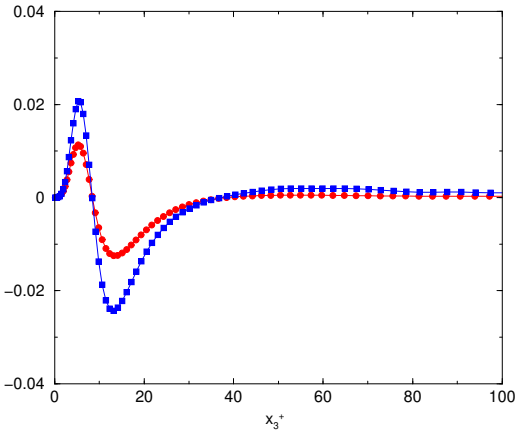

Figure 4: Diffusion of the turbulent energy including the subgrid and resolved scales. $\left\langle J_k^{(s+r)+} \right\rangle$: ■; $\left\langle J_k^{(s)+} + j_k^{(r)+} \right\rangle$: ●.

get the analysis one step further, Figure 4 shows the profiles of the turbulent energy diffusion including the total scales $J_k^{(s)} + j_k^{(r)}$ and $J_k^{(s+r)}$ where $j_k^{(r)}$ is computed from (15). As expected, a relatively good agreement is obtained between these two terms confirming that the diffusion of the resolved scales $j_k^{(r)}$ must be absolutely accounted for in the variational analysis because of its non zero value. Obviously, the same result prevails for the resolved diffusion terms $J_{\epsilon}^{(s)} + j_{\epsilon}^{(r)}$ and $J_{\epsilon}^{(s+r)}$.

4 Conclusion

Variational analysis of the partially integrated transport model has been conducted in a mathematical framework. It has been found that the coefficient $C_{\epsilon_2}^{(s)}$ used in the dissipation-rate equation (8) for $\epsilon^{(s)}$ still verifies a linear dependence in Equation (1) with the subfilter turbulent energy ratio $\left\langle k^{(s)} \right\rangle / \langle k \rangle$ establishing the result in the general case of non-homogeneous flows. The similar result has been found for the coefficient $C_{\epsilon\theta\theta_2}^{(s)}$ used in the dissipation-rate equation (33) $\epsilon_{\theta}^{(s)}$ of the half-scalar variance which also verifies a linear dependence with the ratio $\left\langle k_{\theta}^{(s)} \right\rangle / \langle k_{\theta} \rangle$. The well known fully developed turbulent channel flow has been performed for illustrating the results of the variational calculus. In particular, it has been shown that the resolved turbulent diffusion terms play a significant role in the acting mechanisms of turbulence and cannot be therefore neglected, even if these terms do not explicitly appear in the subfilter model because they are computed from the simulation itself and not modeled.

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