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On general-purpose turbulence models in CFD[2]

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Abstract

The computational fluid dynamics (CFD) tools for various flow problems have become widespread nowadays, yet their use still needs attention and care. In particular, turbulence models are often a crucial part of flow computations undertaken with various software packages, either commercial, open-source or in-house. In the paper, an overview of available model categories is provided, together with some discussion of their advantages or drawbacks with respect to flow cases of interest.

Keywords: Computational fluid dynamics; Turbulence modeling; Reynolds – averaged approaches

1 Introduction

1.1 Motivation and aim

Turbulent regime is dominant in environmental and engineering fluid-flow problems. Since the advent of computational fluid dynamics (CFD), software packages have gained a lot of popularity. On the one hand, their functionalities such as mesh generators, implemented models of the flow physics, options of user-defined functions, numerical solvers and post-processing routines have become increasingly mature, general-purpose and efficient. On

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[2]Dedicated to Professor Romuald Puzyrewski on the occasion of his 80th birthday

the other hand, the CFD tools are in general more and more user-friendly, hence available also for less experienced practitioners. Yet, for an efficient use of CFD packages, a good level of knowledge about flow thermomechanics and numerical methods is a prerequisite.

Over the years, there have appeared various initiatives on CFD tutorials, manuals, guides, user-groups mettings, etc. Among those, the idea of summing-up the experience gathered on various aspects of CFD use and related difficulties in the form of Best Practice Guide seems to be most helpful, see e.g. [4] or specific Internet sites. In particular, attention is needed when it comes to the choice and use of turbulence models [5]. First, because of many variants of such models available, with their inherent complexities and subtleties. These issues include interrelationships with the mesh shape (in particular near the flow boundaries), or even methods of flow solution: the finite volume, now standard, the finite element or other approaches. Second, because new model proposals (or combinations thereof, including physical or zonal hybrid models) continue to appear and are tested for various flow configurations and for physically-complex situations, such as multiphase flows or combustion [2].

Due to the extreme richness and variety of turbulent flows, both in terms of geometrical and physical complexity, there is a general agreement that no single turbulence model, or closure, can be deemed universal, i.e., reasonably suitable for most of typical flow cases. As an introduction to the realm of turbulence and its modeling, the textbooks [7, 16] or more specialized monographs [8, 13] may be referred to. The aim of this paper is to provide a brief overview of turbulence models and to sensitize the CFD users, in particular the less experienced ones, to the advantages and drawbacks of selected available closures with respect to flow cases of interest.

1.2 Fully resolved flow simulations

In turbulent flow, the fields of hydrodynamic quantities such as the velocity $\mathbf{U}(\mathbf{x}, t)$ are tridimensional and unsteady. The approach that consists in solving the complete system of governing flow equations (unsteady, 3D), i.e., continuity, momentum (Navier-Stokes), and possibly energy, is known as fully resolved, or direct, numerical simulation (DNS) [13]. All spatial and temporal flow scales (eddies) are thus resolved, down to the smallest ones, described by the Kolmogorov length scale, η_K, and timescale, τ_K. The computational mesh size should be smaller than η_K and the time step of the simulation should be smaller than τ_K. Given the integral length scale

L (roughly the size of large, energetic eddies) which is close to the system size, and the expression for the Kolmogorov scale [16], the number of mesh nodes in 3D computations can be estimated as $(L/\eta_K)^3 \sim \mathrm{Re}_L{}^{9/4}$ where Re_L is the flow Reynolds number based on the length parameter L. This incurs an extremely high computational cost of the DNS approach and limits its applicability to simple geometries and fairly low Reynolds numbers. On the other hand, the DNS allows for a precise control of flow parameters, and is called 'numerical experiment'. Therefore, DNS plays an increasingly important role in turbulence research thanks to its insight into the flow physics and the structure of turbulence: time evolution of 3D instantaneous fields, multipoint correlations, probability distribution functions, as well as the Lagrangian statistics (hardly available from experiments). The DNS also serves to validate assumptions underlying various turbulence closures through *a priori* analysis and to assess them through *a posteriori* tests [16]; an example of such approach to dispersed flow modeling is [11]. Moreover, DNS is a precious tool to investigate turbulent reactive flows in simple geometries, because a sound description of chemical reactions involves scales of the order of η_K and smaller (molecular mixing) that have to be modeled in other methods.

The fully-developed channel flow with periodic boundary conditions is one of the favourite flow cases of turbulence modellers. It may serve as a reference case to estimate the computational effort of real-life industrial applications such as duct flows or blade-to-blade channels in turbomachinery, etc. In 1987, the first DNS of such a flow was done at $\mathrm{Re}_\tau = 180$ (the Reynolds number based on the friction velocity). Recent results (2014, J. Jimenez group) have been reported in [14]. Using the approximate relationship $\mathrm{Re}_\tau = 0.09\mathrm{Re}^{0.88}$ [16], this corresponds to the channel half-width based Reynolds number of $\mathrm{Re} = 2 \times 10^5$ which is still a way off typical Reynolds numbers encountered in turbomachinery. Moreover, unlike industrial CFD runs based on the second-order discretisation in physical space, the channel flow DNS are most often performed with spectral solvers (except for the wall-normal direction); such approach is extremely fast and accurate. So, extrapolating the growth in computer resources to date, the DNS of duct-like flows of practical interest may probably become feasible in (a few) tens of years only. Simplified approaches to flow turbulence are thus still with a reduced number of degrees of freedom being solved for.

1.3 Rationale for a reduced description of flow turbulence

Strong fluctuations of flow quantities are an intrinsic feature of turbulence, so it is natural to go for a statistical description of the phenomenon. This initiated in 1895 with the seminal paper by O. Reynolds. The description in terms of averaged flow fields is usually limited to the two lowest-order moments: the mean values and the one-point, one-time, second-order correlations. The closure variants are numerous and include algebraic, one-equation, two-equation, and full Reynolds stress models [8]. With the advent and development of DNS and LES approaches, the statistical closure models tend now to get classified into a common category of RANS (Reynolds-averaged Navier-Stokes). This is because the starting point of all these closures is the Reynolds averaging or, alternatively, the density-weighted (Favre) averaging for compressible flows. The majority of the currently used engineering turbulence models belong to the category of RANS.

A well-known specific feature of flow turbulence is that it intensifies the transport processes of mass, momentum and heat. Such an enhancement is of paramount importance and bears consequences for global quantities of direct engineering interest, as the species diffusion, the skin friction or flow losses, and heat transfer. This is readily seen through the averaged momentum equation for incompressible flow

$$\rho\left(\frac{\partial\overline{U_i}}{\partial t}+\overline{U}_j\frac{\partial\overline{U_i}}{\partial x_j}\right) \;=\; -\frac{\partial\overline{P}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu\frac{\partial\overline{U_i}}{\partial x_j}-\rho\overline{u_iu_j}\right)+\rho g_i \;\;, \qquad (1)$$

where the effective viscous term contains now an extra contribution, resulting in increased momentum transport, due to the turbulent stress tensor $\mathrm{R}_{ij}=\overline{u_iu_j}$ or, more precisely, its deviatoric part. (NB: strictly, and dimensionally consistent, the apparent stress is $-\rho\overline{u_iu_j}$). We note that half of the trace of R_{ij} tensor is the turbulent kinetic energy, $k=\mathrm{R}_{ii}/2=\overline{u_iu_i}/2$. The fluid density is ρ, and μ is the dynamic viscosity ($\nu=\mu/\rho$ is the kinematic viscosity). Above, the flow velocity $\mathbf{U}$ and pressure P have been formally decomposed into the mean (or smoothed) and fluctuating (or subfilter) parts: $\mathbf{U}=\overline{\mathbf{U}}+\mathbf{u}$ and $P=\overline{P}+p$, respectively. The averaging is denoted by the symbol $\overline{(\cdot)}$; it can be either statistical or local in space. The statistical (ensemble) average leads to the so-called Reynolds-averaged Navier-Stokes (RANS) closures considered at some length in Section 2. The local weighted average (smoothing) yields the large-eddy simulation (LES) approach, briefly addressed in Section 3.

2 Statistical turbulence models

To characterise the turbulent velocity (at a given point and time instant) at the statistical level, the one-point description involves at least the mean value $\overline{\mathbf{U}}$ and the turbulence intensity (given by k). Since the instantaneous turbulent velocity is always 3D, a more accurate description should involve complete second-order moments $\overline{u_i u_j}$. Moreover, as all models considered in this section use one-point statistics only, some length scale L is needed to provide information about the spatial correlation of the field. Another important quantity in turbulence modeling is a measure of the change-in-time of the turbulent kinetic energy. In particular, because of the cascade character of the energy transfer (from the large to small eddies, and then to heat due to viscous action), a useful and physically meaningful quantity is precisely the dissipation rate of k, called ε [$\mathrm{m}^2/\mathrm{s}^3$].

2.1 Eddy-viscosity closures

First, and possibly the most popular, class of RANS are eddy-viscosity models (EVM) that introduce the effective (turbulent) viscosity, ν_t, based on the Boussinesq hypothesis, to determine the Reynolds stress tensor, R_{ij}, from the linear relationship

$$\mathrm{R}_{ij} = -2\nu_t \mathrm{S}_{ij} + \frac{2}{3} k \delta_{ij} \tag{2}$$

where $\mathrm{S}_{ij} = \left(\partial\overline{U_i}/\partial x_j + \partial\overline{U_j}/\partial x_i\right)/2$ is the mean strain rate tensor. This hypothesis is based on the analogy with the constitutive equation for Newtonian fluid in general fluid mechanics. Some important remarks are in order. The relationship (2) of R_{ij} and S_{ij} involves strong assumptions: it is local, linear, and it contains a scalar proportionality factor ν_t (rather than a 4th rank tensor). Though, there are numerous counter-examples from real-life flows such as a confusor-like (or diffuser-like) flow section followed by a straight duct [16]. The components of the turbulent stresses evolve smoothly downstream, unlike the strain components, and Eq. (2) cannot account for this stress history effect. This obviously undermines the assumption of a local character of Eq. (2) and suggests that differential models, with R_{ij} governed by their evolution equations, are physically better justified.

Also, the constitutive equation for Newtonian flow does not include any dependence on the rotation tensor, since no shear stresses appear in laminar purely rotational flows. However, in turbulent flows with swirl or body

forces due to the system rotation (e.g., a rotor analysed in a relative coordinate system), such as the rotating channel flow, there is a clear dependence of R_{ij} on the system angular velocity. Neither such phenomena, nor turbulence-driven secondary flows in ducts/channels can be correctly predicted by linear EVM of Eq. (2). Hence the idea of non-linear eddy viscosity models (NLEVM) [13] with the explicit dependence also on the mean rotation tensor $\Omega_{ij} = \left(\partial\overline{U}_i/\partial x_j - \partial\overline{U}_j/\partial x_i\right)/2$. Alike, the linearity of the Boussinesq hypothesis, with a scalar proportionality coefficient ν_t, is best verified in thin shear flows with a dominant strain, say $\partial\overline{U}_x/\partial y$, proportional to the shear stress $\overline{u_x u_y}$, such as attached boundary layers, but also jets and wakes. For such flows, Eq. (2) may be thought of as a definition of ν_t. The thin shear flows are of importance in aerodynamic and turbomachinery applications, including flows past slender bodies (profiles, wings, blades, etc.) without separation. Therefore, even simple turbulence closures, such as algebraic or one-equation models, may work fine for such flows. Examples include the mixing-length-like formulae, the one-equation Spalart-Allmaras model for ν_t, etc.

Among the EVM, the two-equation models (for the velocity scale and for the length scale or its equivalent) are widely used, since the closure does not require any input dependent on flow regime or geometry [4]. The turbulent velocity scale, v, is most often found as $v \sim \sqrt{k}$ from the transport equation for the turbulent kinetic energy. Its exact (unclosed) form is readily obtained as half of the trace of the R_{ij} transport equations, see Eq. (6) below. A suitable closure goes through the use of the gradient transport hypothesis of the turbulent diffusion term, resulting in

$$\frac{Dk}{Dt} = \frac{\partial}{\partial x_i}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right] + \mathcal{P} - \varepsilon \tag{3}$$

where D/Dt stands for the material derivative along the mean streamlines and $\mathcal{P}$ is the production rate of the turbulent kinetic energy

$$\mathcal{P} = -\frac{\partial\overline{U_i}}{\partial x_j}\overline{u_i u_j}\,. \tag{4}$$

In EVM, $\mathcal{P}$ is modeled, see Eq. (2); consequently, it is always nonnegative.

As discussed above, the one-point statistical closure has to be supplemented by the length-scale information. It is most often provided by the dissipation rate, ε, of the turbulent kinetic energy k, given by $\varepsilon = \nu\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}}$. Then, since $L \sim v^3/\varepsilon$ for dimensional consistency, the turbulent viscosity

needed in Eq. (2) to close Eq. (1) is found from $\nu_t = C_\mu k^2/\varepsilon$, with a model constant usually taken as $C_\mu = 0.09$.

The transport equation for the dissipation rate contains the small-scale information (the contribution of the smallest eddies to energy dissipation is dominant). Therefore, it is usually closed in an empirical way (the RHS terms of diffusion, production and destruction)

$$\frac{D\varepsilon}{Dt} = \frac{\partial}{\partial x_i}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + \left(C_{\varepsilon 1}\mathcal{P} - C_{\varepsilon 2}\varepsilon\right)\frac{\varepsilon}{k} \tag{5}$$

where C_ε's are model constants. Alternatively, the length scale can be determined as $L \sim v/\omega$ with the turbulent frequency ω $[1/s]$. The ω transport equation, once closed, has a similar structure (production, diffusion and destruction terms on the RHS) as the one for ε. The shear-stress transport (SST) model by Menter with the ω equation improves modeling of flows with separation regions. As the closure for ω has been reported to behave better than the one for ε in the near-wall regions, some eddy-viscosity models link the two, with a switch at certain distance from the wall. Generally, the eddy-viscosity closures have been recalled above in their high-Re form. They use the so-called wall functions to bridge over the viscosity-dominated near-wall region and avoid a fine and costly mesh there. In case of complex geometry or flows with adverse pressure gradients (APG), the wall function approach may lead to inaccurate predictions. The low-Re variants of turbulence models need then to be used [4].

The linear EVM are known to suffer from the overprediction of turbulent energy in regions of high streamline curvature, e.g., upstream of stagnation points [8, 13]. Typical examples are the leading edge zone of a turbine blade, impinging jet, or flow reattachment regions. This modifies the flow downstream through an increased boundary layer thickness, profile losses, etc. Some curative measures with limiters for the production $\mathcal{P}$ have been proposed, see [19]; another option is to use a NLEVM. Akin to it, and promising for some more complex flows, are algebraic Reynolds stress models (not discussed here).

2.2 Reynolds-stress models

Second, and possibly the most advanced, class of RANS are the Reynolds stress models (RSM) where the transport equations for the turbulent stresses are formulated and closed. Other widely-accepted acronyms for RSM exist, such as differential stress model (DSM), second-moment closure (SMC) or

R_{ij}-ε models. The RSM do not use the notion of turbulent viscosity and allow for more physically sound modeling of various flow features, like history effects, swirl, streamline curvature, system rotation and buoyancy [8], as compared with simpler moment closures such as two-equation models (k-ε or alike). Yet, the popularity of RSM in applications remains mitigated because of a higher computational cost and, sometimes, mathematical difficulties with terms being closed.

The turbulent stress tensor $-\overline{u_i u_j}$ plays a central role in statistical turbulence modeling. It appears as an unknown in the Reynolds-averaged momentum equation, Eq. (1), giving rise to the well-known closure problem. According to Launder [8], a rationale for going up to the second-moment closure is the principle of receding influence. The transport equation for R_{ij} is introduced on the premises that imperfections in closure models for higher-order correlations (like $\overline{u_i u_j u_k}$) reflect themselves in errors in the correlations of directly-lower order (like $\overline{u_i u_j}$), but have a limited impact on moments of still lower order (like $\overline{U_i}$). Hence the RSM provides better chances for accurate predictions of the mean velocity field in turbulent flow than eddy-viscosity models.

In the RSM, the components of R_{ij} are treated as new variables governed by their own equations derived from the N-S equation. The transport equation for $\overline{u_i u_j}$ symbolically writes

$$\frac{D\overline{u_i u_j}}{Dt} \equiv \frac{\partial}{\partial t}\overline{u_i u_j} + \overline{U}_k \frac{\partial \overline{u_i u_j}}{\partial x_k} = \mathcal{P}_{ij} + \mathrm{D}^{\nu}_{ij} + \mathrm{D}^{T}_{ij} + \mathrm{D}^{p}_{ij} + \Phi_{ij} - \varepsilon_{ij} \,. \tag{6}$$

In the above equation, $\mathcal{P}_{ij}$ is the production rate of the turbulent stresses by the mean velocity gradients and D^{ν}_{ij} is the viscous diffusion term

$$\mathcal{P}_{ij} = -\overline{u_i u_k}\frac{\partial \overline{U_j}}{\partial x_k} - \overline{u_j u_k}\frac{\partial \overline{U_i}}{\partial x_k} \,, \qquad \mathrm{D}^{\nu}_{ij} = \nu \frac{\partial^2 \overline{u_i u_j}}{\partial x_k \partial x_k} \,, \tag{7}$$

D^{T}_{ij} and D^{p}_{ij} are the turbulent diffusion terms by fluctuating velocity and pressure, defined as follows

$$\mathrm{D}^{T}_{ij} = -\frac{\partial \overline{u_i u_j u_k}}{\partial x_k} \,, \quad \mathrm{D}^{p}_{ij} = -\frac{1}{\rho}\left(\frac{\partial \overline{p u_i}}{\partial x_j} + \frac{\partial \overline{p u_j}}{\partial x_i}\right) = -\frac{1}{\rho}\frac{\partial}{\partial x_k}\left(\overline{p u_i}\delta_{jk} + \overline{p u_j}\delta_{ik}\right), \tag{8}$$

whereas Φ_{ij} is the pressure-strain term and ε_{ij} is the dissipation rate tensor

$$\Phi_{ij} = \overline{\frac{p}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} \,, \qquad \varepsilon_{ij} = 2\nu \overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}} \,. \tag{9}$$

In the Reynolds stress transport equation (6), the production and viscous diffusion terms are exact, Eq. (7), and require no modeling. On the other hand, four RHS terms remain unclosed: D_{ij}^T, D_{ij}^p, ε_{ij}, and Φ_{ij}. Of the four, the pressure-strain term is arguably the most difficult to model.

The Φ_{ij} term is of a purely redistributive nature: since $\Phi_{ii} = 0$, it has no effect on the turbulent kinetic energy balance. It is further decomposed into three contributions, stemming from the three source terms in the Poisson equation for the fluctuating pressure (for this reason, the Φ_{ij} term is non-local and cannot be adequately modeled by local quantities). The three contributions to the pressure-strain term are of differing physical nature, and are usually referred to as the slow term, Φ_{ij}^s, (due to turbulent interactions), the rapid term, Φ_{ij}^r, (due to the interactions of turbulence with the mean shear) and the harmonic (or boundary) term, Φ_{ij}^h, that incorporates the constraints imposed by the boundary conditions

$$\Phi_{ij} = \Phi_{ij}^s + \Phi_{ij}^r + \Phi_{ij}^h \ . \tag{10}$$

Usual hypotheses applied to derive the basic version of closure are: high Reynolds number, local isotropy and quasi-homogeneity of turbulence. These conditions are related to the assumed separation of energy-containing and dissipative scales in the energy spectrum of turbulent motion: no effect of molecular viscosity on large-scale eddies on the one hand, and no direct influence of the mean fields on the dissipative eddies on the other hand.

First, the turbulent diffusion terms D_{ij}^T and D_{ij}^p are to be modeled. The turbulent pressure term D_{ij}^p is often smaller than D_{ij}^T and sometimes neglected. Yet, the two are usually lumped into a single diffusion term D_{ij} and modeled together (by adjusting the C_s constant below) with the generalised gradient diffusion hypothesis as [13]

$$\mathrm{D}_{ij} = \mathrm{D}_{ij}^T + \mathrm{D}_{ij}^p = \frac{\partial}{\partial x_k}\left[\left(C_s \frac{k}{\varepsilon}\overline{u_k u_l}\right)\frac{\partial \overline{u_i u_j}}{\partial x_l}\right] \ . \tag{11}$$

The slow and rapid components of the pressure redistribution term are modeled separately. An ingenious physical insight of Rotta allowed him to propose the closure of the slow redistribution term in terms of the isotropisation of turbulence. This corresponds, in a sense, to the cartoon of vortex stretching cascade where vorticity becomes equally distributed among components through nonlinear interactions. In homogeneous turbulence with no imposed mean strain, Eq. (6) reduces to

$$\frac{D\overline{u_i u_j}}{Dt} = \Phi_{ij}^s - \varepsilon_{ij} \ . \tag{12}$$

It is experimentally observed that such a turbulence tends to the isotropic state. Hence, with the useful definition of the normalised Reynolds stress anisotropy tensor

$$\mathrm{b}_{ij} = \frac{\overline{u_i u_j}}{2k} - \frac{1}{3}\delta_{ij} \,, \tag{13}$$

a linear return to isotropy is written as

$$\frac{D\mathrm{b}_{ij}}{Dt} = -(C_1 - 1)\frac{\varepsilon}{k}\mathrm{b}_{ij} \,. \tag{14}$$

On the other hand, the so-called rapid pressure term Φ_{ij}^r is modeled using hints from the rapid distortion theory (RDT) that analytically determines the evolution of turbulence undergoing fast distortions and predicts the isotropisation of the stress production rate tensor $\mathcal{P}_{ij}$ [16]. The limit cases of slow and rapid distortions are integrated in a following complete picture, known as the basic pressure-strain model of Launder, Reece and Rodi, or LRR-IP model, containing independently the return to isotropy, derived from Eq. (14), and the isotropisation of production (IP):

$$\Phi_{ij} = -C_1\varepsilon\mathrm{b}_{ij} - C_2\big(\mathcal{P}_{ij} - \frac{1}{3}\mathcal{P}_{kk}\delta_{ij}\big) \,. \tag{15}$$

The first and second RHS terms of the basic pressure-strain model, Eq. (15), are referred to as the Rotta model and the IP model, respectively; C_1 and C_2 are model constants [8].

The usual way of closing the dissipation rate tensor ε_{ij} in Eq. (6) goes through the Kolmogorov assumption of locally isotropic turbulence at high Reynolds numbers: due to the fact that dissipation occurs mainly at small flow scales this tensor is to a good approximation isotropic, $\varepsilon_{ij} = (2/3)\varepsilon\delta_{ij}$.

In near-wall regions, the RSM need to by complemented by low-Re modifications. One of the reasons is the existence of the wall-reflection terms in pressure-strain correlations. An alternative to *ad hoc* damping formulae has been the elliptic blending approach, still being improved in RSM closures [14], and successfully developed also in PDF method for near-wall flow solution [20].

The RSM, as other one-point statistical closures, needs the length-scale equation, or its equivalent. This is provided by the dissipation rate ε of the turbulent kinetic energy k, already introduced in Section 2.1. It is a scalar resulting from the contraction of the dissipation rate tensor ε_{ij}, present in RSM equations:

$$\varepsilon = \frac{1}{2}\varepsilon_{ii} = \nu\overline{\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}} \,. \tag{16}$$

The closure of the ε transport equation is similar as in the eddy-viscosity models, discussed before.

Finally, the complete set of RSM equations in its basic (high-Re) version consist of the mean continuity, momentum, Eq. (1), the Reynolds stress transport, Eq. (6), with adequate models for unclosed RHS terms, and the transport equation for a time scale (or for the dissipation rate ε).

2.3 PDF methods

Roughly speaking, difficulties about the statistical modeling of turbulence are twofold: nonlinearity and nonlocalness. The nonlinearity manifests itself in the convective term of the N-S equations and is still present in the Reynolds equations for the mean velocity as well as in the transport equations for higher-order moments. Moreover, in chemically reactive flows (combustion), the source terms in species conservation equations are usually highly nonlinear.

The probability density function (PDF) approach remains statistical. Yet, unlike EVM or RSM that resolve the moments of the velocity (the mean field and, at most, the second-oder moments R_{ij}), the PDF method is based on the transport of the one-point probability density of velocity [16]. In the PDF method, contrary to the RANS moment approaches, there are no problems due to nonlinearity. The convective terms are exact thanks to the Lagrangian description and the source terms in the scalar transport equations (if any) are exact thanks to introducing the species mass fractions into the PDF; hence, no modeling is needed. At the level of the PDF equation, the linearisation has been achieved at the expense of increasing the number of independent variables (e.g., velocity). However, the remaining major difficulty for both the PDF method and the moment closures (like RSM) is the modeling of non-local effects that remain unknown in the one-point description.

The departure point for the stochastic modeling of turbulence are the trajectory equations (advection in physical space and the momentum equation):

$$dx_i = U_i\,dt \tag{17}$$

$$dU_i = \left(-\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i} + \nu\frac{\partial^2 \overline{U_i}}{\partial x_j \partial x_j}\right) dt + \left(-\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j}\right) dt\ . \tag{18}$$

Contrary to the moment closures where the point of departure is the Reynolds equation, Eq. (1), in the PDF approach the closure is applied directly at

the level of instantaneous flow variables. This is usually done with the use of stochastic diffusion processes. The closure strategy, including also heat transfer modeling, has been presented in [17]. The main idea is to replace the exact instantaneous equations by modeled instantaneous ones. In particular, a high-Reynolds model for the Navier-Stokes equation has the form [16]:

$$d\mathcal{X}_i = \mathcal{U}_i\, dt, \tag{19}$$

$$d\mathcal{U}_i = -\frac{1}{\rho}\frac{\partial \overline{P}}{\partial x_i}dt + \mathrm{G}_{ij}(\mathcal{U}_j - \overline{U_j})dt + \sqrt{C_0\varepsilon}\, dW_i, \tag{20}$$

where C_0 is a constant and $\boldsymbol{\mathcal{U}}(t)$ is the velocity of a stochastic particle, defined as the Eulerian fluid velocity $\mathbf{U}(\mathbf{x}, t)$ evaluated at the particle position, i.e., $\boldsymbol{\mathcal{U}}(t) = \mathbf{U}\,[\boldsymbol{\mathcal{X}}(t), t]$. It is readily seen that advection in Eq. (19) is exact, the mean viscous term in Eq. (20) has been neglected and the sum of the fluctuating terms (pressure gradient and diffusion of momentum) has been replaced by a stochastic process of the diffusion type. The drift matrix G_{ij} is assumed to be a function of local mean variables, such as $\overline{u_i u_j}$, $\partial\overline{U_i}/\partial x_j$, ε, etc.; various models have been proposed, some of them in relationship with the Reynolds-stress equations. The closed trajectory equations, Eqs. (19)–(20), form a system of stochastic differential equations (SDEs) and are solved with the Monte Carlo method.

For the stochastic description to be self-contained, the values of the mean dissipation rate, ϵ, at the particle locations are needed, cf. Eq. (20). This can be done with a standard modeled PDE for ε, solved on a grid and interpolated at particles. An alternative way, consistent with the stochastic approach, goes through actually writing a model for the instantaneous dissipation rate (or the turbulent frequency) along particle paths. Information on the instantaneous dissipation not only gives access to the mean value but also allows for the internal and external intermittency of the flow to be directly simulated [17].

The PDF approach is more often used for computation of reactive flows where it is applied to scalar variables (like the species mass fractions) whereas the flow variables are found from a standard CFD RANS solver. This results in a hybrid approach with a physical coupling of the two sets of variables. The are some consistency issues; yet, the scalar PDF method (recently, also coupled to LES solvers) offers an advantage of exact computation of species source terms and is suitable to all classes of reactive flows (diffusion, premixed, partly premixed), also with complex chemical kinetics.

3 Other closures, alternative solvers

3.1 Large eddy simulations

In the large eddy simulations (LES) setting [16], the averaging operator $\overline{(\cdot)}$ represents *de facto* a filter, hence Eq. (1) can be thought of as a smoothed N-S equation where the small-scale instantaneous flow structures are filtered out but the unsteady character of turbulent flow (in the sense of large-scale instantaneous fields) will be preserved.

The idea of the LES approach is based on the assumption of the cascade transport of turbulent energy, generated at the length scales, L, corresponding to the largest flow structures, transported to smaller eddies through nonlinear vortex interactions, down to the viscous dissipation at the smallest scales. Physically, the filtering process removes the eddies smaller than the filter size Δ. In practice, Δ is the characteristic size of grid cells. The removed part of the turbulent spectrum is called the sub-grid scale (SGS) part. The filter size is chosen to solve a considerable part of the turbulent kinetic energy of the flow at an acceptable cost of computations. In LES, the filtering operator is defined as the convolution with the filter G

$$\overline{U}_i = G * U_i \ , \quad \overline{U}_i(\mathbf{x},t) = \int G(\mathbf{x}-\mathbf{x}',t)U_i(\mathbf{x}',t)d\mathbf{x}', \tag{21}$$

and the filtered transport equations have the same structure as the Reynolds equation.

Applying the SGS viscosity hypothesis (analogous to the Boussinesq hypothesis in RANS), the deviatoric part of the SGS stress tensor, here $\tau_{ij} = \overline{U_iU_j} - \overline{U}_i\overline{U}_j$, is assumed proportional to the resolved strain rate $\overline{\mathrm{S}}_{ij} = (\partial\overline{U}_i/\partial x_j + \partial\overline{U}_j/\partial x_i)/2$ as

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\nu_{sg}\,\overline{\mathrm{S}}_{ij} \ . \tag{22}$$

The SGS viscosity may be found as the product of suitable length and velocity scales, i.e., $\nu_{sg} \sim l_m v_m$, where $l_m \sim \bar{\Delta}$ and $v_m \sim l_m|\overline{\mathrm{S}}|$:

$$\nu_{sg} = C_G\bar{\Delta}^2|\bar{S}| \ ; \tag{23}$$

C_G is a model coefficient and $|\overline{\mathrm{S}}| = (2\overline{\mathrm{S}}_{ij}\overline{\mathrm{S}}_{ij})^{1/2}$ is the scalar strain rate based on the second invariant of $\overline{\mathrm{S}}_{ij}$. Despite many variants of SGS models proposed to date, this reamins an open reserch issue, in particular for physically-complex flows.

The LES approach is particularly well suited for free shear flows and other flow configurations whose dynamics is dominated by large structures (jets, flows past bluff bodies, wake-blade interactions, etc.). Unfortunately, LES becomes quite expensive when it comes to wall-bounded turbulence, since the near-wall vortical structures, crucial for a correct resolution of the turbulent boundary layer, are small compared to those in the core. Therefore, LES with wall functions and hybrid RANS-LES approaches are often considered for the sake of efficiency. Yet, in general, thanks to the modeling of small eddies only (rather than the whole spectrum) the LES closures are simpler than the elaborate RANS variants and the instantaneous flow fields are better simulated. These features, together with the continuing growth of computer technology, make the LES approach increasingly popular in engineering CFD applications.

3.2 Alternative methods: SPH, LBM

This section briefly addresses some new approaches for flow computation, or solvers, alternative to the 'mainstream' CFD where finite volume or finite element methods are most often used. Notwithstanding the solver, the issue of turbulence modeling remains and needs considerable attention.

Smoothed particle hydrodynamics (SPH) is a Lagrangian (particle) approach, where the flow dynamics is represented by a (large) number of coupled ordinary differential equations for particles' advection and the evolution of suitable quantities carried on by the particles (momentum, energy, phase indicator, etc.) [19]. The approach is not (yet) used in the mainstream CFD. However, it has already found some application areas, such as free surface flows, two-phase flows with complex interfaces, problems involving fluid-structure interactions (FSI), including/or the computation of solid mechanics with material rupture, etc. One of the SPH advantages is its meshless nature, avoiding thus the time-consuming grid generation for complex geometries. This advantage becomes however a drawback when a spatially-variable resolution or adaptive refinement are needed. SPH has recently been applied to turbulent flows, with a mixed success [15]. Also, a variant of SPH has been dealt with in [6] to simulate a generic free-shear flow (turbulent mixing layer) using a particle-based LES.

For several years now, flow solvers based on the lattice-Bolzmann method (LBM) have gained a lot of attention because of their computational advantages. In LBM, unlike the classical CFD approaches based on the solution of the macroscopic flow equations, the departure point is the Boltzmann

equation discretised in physical space, time, and in the velocity space. For a summary of the LBM capabilities, including turbulent and other complex flows, a review paper [1] and references therein may be referred to. On the advantageous side of LBM, even complex geometries are usually discretised using a regular grid with a suitable implementation of boundary conditions. This saves human effort, since the tedious meshing is no longer necessary. Moreover, the LBM solvers are very efficient and readily subject to high performance computing with massively parallel clusters or GPU (graphics processing units) technology. On the other hand, the implementation of more complex physics, such as chemical reactions or heat transfer [9], is not straightforward. A recent paper [18] is a representative example of LBM used for engineering flow studies (a water pump intake with the transient vortex). Another example of LBM application to turbulent flow case, together with some comparisons to the finite-volume and SPH method is the work [10].

3.3 Flow design

There is a lot of practical interest to apply CFD tools to the flow design problem. Most often, flow design is formulated in terms of the optimisation task that usually needs many time consuming solutions of the simple (or analysis) flow problem. A demanding option goes through the reformulation of the Reynolds equation (with a suitable turbulence model) to the stream line coordinate system [3]. In practice, a whole new solver has to be written, but this makes it possible to formulate an inverse problem and solve it in a single shot, at least for a preliminary design. This allows one to accelerate a tedious optimisation procedure, where each iteration step requires a flow solution. The flow design may also be achieved in a hybrid approach where an inverse method based on some assumptions about the streamline shape (e.g., in turbomachinery) is coupled with the standard CFD flow analysis that provides data on flow losses [12].

4 Conclusion and perspectives

The variety of turbulence models developed to date is impressive. In the paper, a brief overview of some classes of closures has been made, including in particular the two-equation eddy-viscosity models, RSM closures and LES, because of their importance or future potential. Despite their widespread

availability in CFD software packages, turbulent models are sometimes applied by less-experienced users without due attention (in the 'black-box' mode). This may result in inaccurate predictions (sometimes even completely wrong) or inefficient use of CFD tools.

The two-equation models are probably the most often used by CFD practitioners, partly because of their 'general-purpose' flavour. Yet, for particular applications, such as the streamlined flows in aerodynamics and turbomachinery, even some simpler one-equation closures may work fine. On the other hand, the Reynolds stress transport equations are definitely more suitable for flow cases involving high streamline curvature, buoyancy effects, or flows in rotating systems. For that class of flows, nonlinear EVM or algebraic RSM are also used.

Apart from the classical CFD solvers and their application for flow analysis, alternative methods are developed and other areas of interest, such as flow design, are explored. Also, new ideas for more efficient, or more detailed, modeling of turbulent flows still appear. In the current CFD practice, progress in available computing power causes already a shift from RANS-based closures towards LES and hybrid approaches. Still, especially for the analysis of complex turbulent flows (in terms of multiphysics or geometry), an expert knowledge and skills of CFD users are required for success.

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