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Turbulence, from stochastic to deterministic approach

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Abstract

The paper presents contemporary development in the field of deterministic description of turbulence with a special reference to Large Eddy Simulation (LES) methods. The limitations of conventional turbulence modelling based on stochastic methodology have been discussed and reasons for the development of deterministic approach have been outlined. It has been shown that the computational power of the fastest available computers restrict the possible DNS (Direct Numerical Simulation) solutions to the range of small Reynolds numbers. Finally, the basic assumptions have been formulated for the LES formalism, that seem to offer the reasonable compromise between the tendency towards the deterministic solution of Navier-Stokes equations and the existing computational resources.

Keywords: Turbulence; CFD; Large Eddy Simulation

Nomenclature

- C_s – constant in Smagorinsky model
- D_{ij} – mean rate of strain tensor
- F – arbitrary physical quantity – mass force Eq. (3)
- f – fluctuating component of arbitrary physical quantity
- G – filter for N-S equation
- k – kinetic energy of turbulence
- L – macroscopic dimension of the flow
- S – rate of strain tensor for filtered flow-field
- U_i – instantaneous velocity component
- u_i – fluctuating component of velocity
- $\mathbf{x}$ – space vector
- x_i – space coordinates
- α – coefficient in eddy viscosity definition
- Δ – subgrid length scale
- δ_{ij} – Kronecker delta
- ε – turbulence energy dissipation
- η – Kolmogorov scale
- ν – kinematic viscosity coefficient
- ν_T – eddy viscosity
- σ_{ij} – stress tensor
- ρ – density
- τ_{ij} – subgrid stress tensor
- $(-)$ – time averaging operator
- $(=)$ – filtration operator
- $(*)$ – convolution

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1 Introduction

Turbulence in viscous flows presents the most common and also the most complex flow both in natural environment and technical applications. The most important feature of these flows is the existence of vortex structures featuring the length scales continuously varying from the smallest one of the order of 10^{-6} m up to macroscopic dimensions of the flow equal to hundreds and sometimes even thousands of kilometers [1]. The first consequence of such a turbulence structure is the infinite number of interactions among particular eddy scales which introduce the need of stochastic description of turbulence. In this methodology one does not try to describe the behaviour of individual eddies but instead of this considers statistically averaged measures which characterise turbulent eddies and turbulence structure. One should remember however, that the trustworthy description of eddy structure requires averaging of a considerable number of particular flow realisations. Equally important consequence of the existence of eddy structure is the enormous intensification of both mixing processes and transport abilities which result from the infinite number of interactions between particular eddies in the turbulent flow.

Summing up, one may conclude that the correct description of turbulent flow must on the one hand reflect the existence of infinite eddy cascade and on the other hand it must account for the intense mixing and transport properties as the important feature of turbulence.

2 Stochastic turbulence modelling

The stochastic treatment of turbulent flow became possible due to the idea of O. Reynolds, who assumed that each physical quantity F, which characterizes the flow turbulence, may be treated as a superposition of a time invariant mean quantity $\overline{F}(\mathbf{x})$ and a fluctuating component $f(\mathbf{x},t)$ being a random function of space and time:

$$F(\mathbf{x},t) = \overline{F}(\mathbf{x}) + f(\mathbf{x},t)\,. \tag{1}$$

Application of the above hypothesis allows to describe the velocity field $U_i(\mathbf{x}_j,t)$, pressure $p(\mathbf{x}_j,t)$ and density $\rho(\mathbf{x},t)$ as a following superposition:

$$\begin{aligned} U_i(x_j,t) &= \overline{U_i}(x_j) + u_i(x_j,t) \\ p(x_j,t) &= \overline{p}(x_j) + p'(x_j,t) \\ \rho x_j, t &= \overline{\rho}(x_j) + \rho'(x_j,t) \end{aligned}\,. \tag{2}$$

If one introduces the above relations to Navier-Stokes equations, then for incompressible flow ($\rho = \overline{\rho} = idem$) of constant viscosity fluid ($\nu = idem$) the Reynolds equation may be written:

$$\rho\left(\frac{\partial \overline{U_i}}{\partial t}+\overline{U_j}\frac{\partial \overline{U_i}}{\partial x_j}\right)=\frac{\partial}{\partial x_j}(\sigma_{ij})+\overline{F_i}\,. \tag{3}$$

The above equation is time-averaged which is equivalent to averaging over infinite number of realisations of stochastic process. The stress tensor from the above equation:

$$\sigma_{ij}=-\overline{p}\delta_{ij}+\frac{\nu}{\rho}\left(\frac{\partial \overline{U_i}}{\partial x_j}+\frac{\partial \overline{U_j}}{\partial x_j}\right)-\rho\overline{u_i u_j}\,, \tag{4}$$

contains an additional term:

$$(\sigma_T)_{ij}=-\rho\overline{u_i u_j}\,, \tag{5}$$

which was not present in the original Navier-Stokes equation. This additional term is the symmetric, second order turbulent stress tensor commonly called the Reynolds stress tensor. The diagonal components of the above tensor, i.e.:

$$-\rho\overline{u_i u_j}$$

represent the normal stress components, while the non-diagonal ones

$$-\rho\overline{u_i u_j}(1-\delta_{ij})$$

are the shear components of Reynolds stresses.

Since the additional stress tensor has appeared, then Reynolds equations are no longer closed. The closure of Reynolds equation requires first of all a proposal concerning the mutual relation between the Reynolds stress components and physical quantities characterizing the mean flow field. Such a concept was given by Boussinesq, who proposed a simple linear relation between the Reynolds stress tensor and the mean flow rate of the strain tensor, i.e.:

$$-\rho\overline{u_i u_j}=\rho\nu_T\left(\frac{\partial \overline{U_i}}{\partial x_j}+\frac{\partial \overline{U_j}}{\partial x_i}\right)\,. \tag{6}$$

The proportionality coefficient ν_T, which appears in the above relation, is the kinematic turbulent viscosity and may be treated as analogy to the Newton viscosity. One should notice, however, that contrary to Newton's idea ν_T is no longer a physical property of the fluid, but it is a property of turbulent flow which depends on the turbulence structure at a given point. The Boussinesq concept enables the analytical treatment of turbulent flow, but it is not a closure of the Reynolds equation, because it does not suggest at all, how the turbulent viscosity could be determined. According to the original Boussinesq idea, the turbulent viscosity ν_T was to be a scalar quantity, determined experimentally as a function of space coordinates, i.e.:

$$\nu_T = \nu_T(x) ,$$

that was meant to enable the formulation of missing relations between turbulent stress and rate of strain tensors. However, such a closure can not be performed for the turbulent flow, because the eddy viscosity is a function of the flow-field which is not known *a priori*. Furthermore, the assumption concerning the scalar behaviour of eddy viscosity was also a matter of serious controversies and as it was pointed out by many authors, (e.g. Hinze [2]), the eddy viscosity should rather be a second order tensor given by the formula:

$$-\rho\overline{u_i u_j} = (\nu_T)_{ik}\overline{D_{jk}} , \tag{7}$$

where $\overline{D_{jk}}$ is the mean rate of strain tensor

$$\overline{D_{jk}} = \frac{\partial \overline{U_j}}{\partial x_j} = \frac{\partial \overline{U_k}}{\partial x_j} .$$

This improved proposal is however not entirely correct, because as it has been pointed out by numerous sources (see for example Elsner [1]) it does not fulfil the basic assumptions concerning the 3D character of turbulent fluctuations. This limitation can be lifted if Eq. (7) is expressed in the form:

$$-\overline{u_i u_j} = \frac{1}{2}\left\{(\nu_T)_{ik}\overline{D_{kj}} + (\nu_T)_{jk}\overline{D_{ki}}\right\} - \alpha_{ij}k , \tag{8}$$

where $k = \overline{u_i u_j}$ denotes the kinetic turbulence energy and coefficient α_{ij} takes the following values:

$$\begin{cases} \alpha_{ij} = 0 & \text{for } i \neq j \\ \alpha_{ij} \neq 0 & \text{for } i = j \end{cases} .$$

The first term of the r.h.s. of Eq. (8) has been written in the form which provides the symmetry of $\overline{u_i u_j}$ tensor indices with respect to i and j. The second term is related to kinetic turbulence energy and takes into account the presence of normal components of turbulent stresses, which have non-zero value even in homogeneous flows, where the mean rate of strain tensor is equal to zero. One should notice however, that introduction of eddy viscosity expressed as second order tensor is not a closure of Reynolds equations, but it only illustrates the complexity of the problem.

These closure hypotheses, which were developed so far and are commonly called the eddy viscosity turbulence models, are mostly based on the idea of scalar eddy viscosity. Within this group of closures one may distinguish algebraic (zero-order) as well as one and two-equation turbulence models, with $k - \varepsilon$ turbulence model developed at the beginning of 70's and most widely used so far [3]. Despite the fact, that many spectacular successes have been achieved with eddy-viscosity models, there is a common knowledge of their inherent limitations resulting e.g. from the assumed scalar character of eddy-viscosity. Understanding these limitations was the reason why at the very beginning of turbulence modelling era, the idea of stress transport models, which does not use the eddy-viscosity concept, was proposed by Hanjalic [3]. Stochastic turbulence models were intensively investigated during 70's and 80's and now a selection of excellent books on that subject is available starting from the classical (although a bit outdated) book by Wilcox [4] and ending with the recent monography by Pope [5].

During 90's the knowledge about turbulence modelling was utilized in the development of commercial codes, which despite their obvious drawbacks are at present the only available tools for analysis of turbulent flows. These complex software packages based on the classical turbulence models solve the time-averaged equations of motion and are widely known as RANS codes (Reynolds Averaged Navier Stokes equations). However, the limitations of RANS codes are not known *a priori* and that is why the analysis of their applicability to various types of flows and evaluation of achievable accuracy of computations is so important that it has been made a subject of currently running EU project known under the acronim QNET-CFD [6]. The obvious motivation for this analysis is the limited versatility of both eddy-viscosity based and stress transport turbulence models. This limitation results directly from time-averaging of N-S equations that requires the ability of turbulence models to cope with the whole range of eddy scales encountered in all possible types of turbulent flows. Many decades of intense research did not allow to develop a truly universal turbulence model [7] and unfortunately a pessimistic forecast of J. Ferziger [8] formulated as early as at the end of 70's seems to be true so far. The research performed currently in this field proposes no more than only minor modifications to already existing turbulence models which result at most in slight improvements of computational accuracy in selected types of flows. One may conclude therefore, that stochastic turbulence models which are now used as the closure for Reynolds averaged N-S equations should not be regarded as a promising perspective. On the other hand the urgent need for CFD design tools, which is evident in all fields of engineering, requires the fluid mechanics research to find a new solution, which could bring a real breakthrough in CFD and which should propose a trustworthy description of turbulent flow [9].

3 New perspectives for deterministic turbulence modelling

The research performed during the decade of 90's revealed that contrary to previous expectations, the N-S equations are capable to describe correctly the structure of turbulent flow in ranges of Reynolds and Mach numbers which are potentially interesting from the engineering point of view. As it was stated by Lesieur [10], there are simple, good quality solutions of N-S equation for very high Mach numbers (M$\approx$ 15), which were obtained at grids with mesh sizes smaller than viscous Kolmogorov scales, but still these sizes are much larger than the molecular free-path. If such a solution gives correct values of velocity, pressure, temperature and density of the flowing medium, then it seems logical to put forward a question concerning the mutual relation between the flow turbulence and Newton's determinism. Bearing in mind the flow physics, this important question may be formulated as follows:

".....if at the initial time-instant t_o one knows the initial positions and velocities of all scales of motion, then there should be only the one possible state of flow for every time instant $t > t_o$".

From the point of view of a mathematician, this question concerns the problem of existence and uniqueness of solution for the N-S equation, which so far has only been proved for the 2D space [11], while in the 3D space the N-S solution exists only for a finite time. There seems to be, however, a reasonably justified hope (see Lesieur [10] among the others) that the presence of viscosity in the N-S equation will tend to 'smooth' the solution at the degree, which will be sufficient to prevent singularities and bifurcations to another solution [12].

The above statements suggest the possibility of deterministic treatment of turbulence even if the solution resulting from the non-linear interactions among the particular scales of turbulent motion will reveal a very complex behaviour. The perspective for analytical N-S solution is of course unrealistic, but the impressive progress in computational resources enables us to obtain numerical solutions of true N-S equation, at least, for the moderate Reynolds numbers. This type of solutions known as DNS (Direct Numerical Simulations) is simply a direct solution of N-S equation obtained in time domain with all scales of turbulent motion accounted for. DNS solution does not require any hypotheses or turbulence models and consecutive DNS solutions, obtained in the time domain are equivalent to particular realisations of stochastic process. One may notice therefore the fundamental advantage of DNS approach, which avoids averaging of equations and replaces this drawback by correct averaging of process realisations that finally leads to statistic measures characterising the flow-field considered.

The next advantage of DNS method is its ability to reproduce correctly the whole range of linear and time scales of turbulence motion, because the eddy cascade is a resolved quantity and not a modelled one. However, one must be aware that this DNS feature is also its basic limitation, if the amount of computational effort is to be considered. The largest scale, comparable with macroscopic flow dimension is of the order

$$L = k^{3/2}/\varepsilon \tag{9}$$

where ε is the viscous energy dissipation and this scale determines the size of computational domain.

If one intends to resolve correctly the turbulence structure, then the mesh size of computational grid should be of the order of smallest eddy scales, which for most applications correspond to the Kolmogorov scale, i.e.:

$$\eta = (\nu^3/\varepsilon) \tag{10}$$

Turbulence is inevitably a 3D phenomenon, so if one takes into account relations (9) and (10), then the number of grid nodes needed for correct DNS solution may be evaluated as:

$$N_{DNS} \approx \mathrm{Re}^{9/4} \tag{11}$$

For typical technical applications the Re number is of the order of $10^4 \div 10^6$, and for geophysical flows it may even be as large as $10^7 \div 10^8$, so the number of nodes calculated from Eq. (11) is enormous and the same is the capacity of computer memory needed for accurate DNS solution. The most powerful computers, which exist nowadays, enable to obtain DNS solutions for turbulent flows characterized by the Re number:

$$Re \approx 10^3$$

which is certainly not sufficient for the most practical applications. Summing up, DNS is the most promising perspective in research aimed at the development of methods enabling the most accurate description of turbulent flows. However, one should also be aware that the distant time horizon needed for effective application of DNS approach is not solely determined by the development of computing power. There is still a gap in our knowledge concerning the dynamics of the smallest scales of turbulence as well as formulation of initial and boundary conditions.

4 Large Eddy Simulation as a perspective for turbulence analysis

Large Eddy Simulation (LES), originally proposed in 1963 for modelling of atmospheric flows [13], was for the first time successfully applied to industrial flow as early as in 1970 [14]. The basic assumption of LES method is the separation of the continuous spectrum of eddy scales into the resolved (i.e. computed) and modelled scales. It means that turbulent flow quantities like velocity, pressure etc. are computed for scales comparable to mesh size of the computational grid, while the same quantities resulting from scales smaller than the mesh size are being modelled. This assumption reflects correctly one of the basic features of turbulence i.e. the tendency towards isotropy in small scales, that allows to expect a much better chance for reliable modelling within this range of scales. On the other hand, the anisotropy, which prevails in larger scales, may properly be resolved in LES computed solution, provided of course that a properly universal subgrid turbulence model may be found.

The separation of scales is achieved by the filtration performed with the use of $G(\mathbf{x})$ filter, that allows to transform the arbitrary flow-field quantity $\overline{F}(\mathbf{x})$, which then is being resolved numerically. The filtration procedure may be written as a convolution, which for simple one-dimensional case may written as:

$$\overline{\overline{F}}= G(\mathbf{x}) * F(\mathbf{x}) = \int\!\!\!\int\!\!\!\int_{-\infty}^{+\infty} G(x-\xi)F(\xi)d\xi \tag{12}$$

where symbols $(=)$ and $(*)$ denote the result of filtration and convolution operator respectively.

Application of the above filtration procedure to N-S equations transforms them into the following form:

$$\frac{\partial \overline{\overline{U}}_i}{\partial t} + \frac{\partial(\overline{\overline{U}}_i\overline{\overline{U}}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{\overline{P}}}{\partial x_j} + \frac{\partial}{\partial x_j}\left\{\nu\left[\frac{\partial \overline{\overline{U}}_i}{\partial x_j} + \frac{\partial \overline{\overline{U}}_j}{\partial x_i}\right] - \overline{\overline{\tau}}_{ij}\right\} \tag{13}$$

where one may notice the appearance of the so-called subgrid stress tensor $\overline{\overline{\tau}}_{ij}$ which is given by the formula:

$$\overline{\overline{\tau}}_{ij} = \overline{\overline{U_iU_j}} - \overline{\overline{U}}_i \cdot \overline{\overline{U}}_j \tag{14}$$

The results obtained by Ferziger and Vreman [8, 15] reveal that subgrid turbulence contains 20-30% of total kinetic energy of velocity fluctuations. If one recalls the tendency towards isotropy in small scales, then both these facts confirm that the chance of successful modelling of subgrid turbulence is certainly larger than in the case of classical RANS approach.

The review of the state-of-art in the field of subgrid modelling has been given recently by Domaradzki [16], Lesieur and Metais [17] as well as by Jimenez and Moser [18]. However, the amount of valuable results obtained in this field is too large to make even a brief summary. Nevertheless, let us try to present at least a classification of subgrid models based on the proposal given by Domaradzki [16], who distinguished three main groups of subgrid models, i.e.:

- viscosity-based models,
- mixed models,
- dynamic models.

The viscosity-based models utilise the Boussinesq concept, transformed [17] as follows:

$$\overline{\overline{\tau_{ij}}} = \overline{\overline{\nu_t}}\,\overline{\overline{S_{ij}}} + \frac{1}{3}\tau_{ll}\overline{\overline{S_{ij}}} \tag{15}$$

where τ_{ij} denotes the subgrid stress tensor given by Eq. [14], $\overline{\overline{\nu_t}}$ is the subgrid eddy viscosity coefficient, while the expression:

$$S_{ij} = \frac{\partial\, \overline{\overline{U_i}}}{\partial x_j} + \frac{\partial\, \overline{\overline{U_j}}}{\partial x_i} \tag{16}$$

is the rate of strain tensor of filtered flow field. The first subgrid closure was proposed by Smagorinsky [13], who developed the subgrid analogy to mixing length model, given by the following formula:

$$\overline{\overline{\nu_t}} = (C_s \cdot \Delta)^2 \cdot |\,\overline{\overline{S}}\,| \tag{17}$$

where Δ denoted the characteristic subgrid length scale, C_s was a constant adjusted arbitrarily for a given flow type (solution), while the absolute measure of local strain was given by the formula:

$$|\overline{\overline{S}}| = \left\{2 \cdot \overline{\overline{S_{ij}}} \cdot \overline{\overline{S_{ij}}}\right\}^{1/2} \tag{18}$$

Despite 40 years which passed since Smagorinsky proposed his model, it is still being used due to its simplicity and highly dissipative behaviour, which stabilizes the computation process. Smagorinsky model reveals also some serious limitations, and among them one should mention at first too large value of subgrid eddy viscosity $\overline{\overline{\nu_t}}$ in the vicinity of walls, that requires some arbitrary correcting functions. Furthermore, it is difficult to propose a sound physical explanation for the proper value of the characteristic subgrid length scale Δ (see Eq. 17) and that is why this important parameter has to be selected in an arbitrary manner. Finally, Smagorinsky model is not able to predict correctly the laminar-turbulent transition process, which is due to its dissipative behaviour. However, the simplicity of this idea was the reason for its development which was especially successful at LEGI Grenoble, where a series of valuable ideas have been proposed. Among the most successful proposals and improvements of original Smagorinsky idea, the following seem to be the most valuable:

- Structure Function Model by Metais and Lesieur [19],
- Selective Structure Function Model by David [20],
- Filtered Structure Function Model developed by Ducros [21].

One should also notice the group of models based on spectral formulation by Kraichnan [22] which were discussed in detail in [10, 17], as well as the interesting generalization of Smagorinsky model, which was presented as HS (Hyper Smagorinsky) model by Jimenez and Moser [18].

Mixed models have been originally proposed by the famous research group at Stanford University [24] and this type of closure together with the dynamic model proposed by Germano [25] are not models in the traditional sense. In fact, both mixed and dynamic models are rather complex algorithms, which try to relate the subgrid stresses with scales of resolved motion [26].

Variety of subgrid models developed so far is on the one hand a proof of the importance of this branch of CFD, but on the other hand it is also a sign of its weakness. In particular, none of the models developed so far seems to be versatile enough to provide a correct description of turbulence structure in various flow types. Nevertheless, both the older [27] and the more recent [29, 30] reviews of the subject prove, that subgrid modelling is still a key issue for further development of LES technique.

5 Summary

Brief description of current trends in turbulence modelling proves the important role of deterministic approach. Both DNS and LES techniques do not, however, continue the trends developed by traditional RANS modelling, but in fact both these approaches are novel treatments of turbulence closure problem. The DNS method is the ultimate goal in this field, but for the time being the still limited computational resources suggest the important role of LES which presents a reasonable compromise between the accuracy of solution and demand for computational effort.

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