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SOME REMARKS ON MODELLING AND SIMULATION OF TURBULENCE[1]

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

Key words: turbulence, RANS, LES, DNS

Notations

C_s	–	constant in Smagorinsky model
D_{ij}	–	mean rate of strain tensor
F	–	arbitrary physical quantity
f	–	fluctuating component of arbitrary physical quantity
G	–	filter for N-S equation
k	–	kinetic energy of turbulence
L	–	macroscopic dimension of flow
S	–	rate of strain tensor for filtered flow-field

[1]The paper was addressed to researches presenting a wide range of fields of their interest at XXXII Meeting of Polish Society Of Theoretical and Applied Mechanics.

U_i	–	instantaneous velocity component
u_i	–	fluctuating component of velocity
$\boldsymbol{x}$	–	space vector
x_i	–	space coordinates
α	–	coefficient in eddy viscosity definition
$\varDelta$	–	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

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 ones of the order of 10^{-6} m up to macroscopic dimensions of flows equal to hundreds and sometimes even thousands of kilometers (Elsner, 1987). The first consequence of such a turbulence structure is an infinite number of interactions among particular eddy scales which introduce the need for stochastic description of turbulence. In this methodology one does not try to describe the behaviour of individual eddies but instead considers statistically averaged measures which characterise turbulent eddies and the turbulence structure. One should remember, however, that trustworthy description of an eddy structure requires averaging of a considerable number of particular flow realisations. Equally important consequence of the existence of an eddy structure is 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 a correct description of a turbulent flow must, on one hand, reflect the existence of the infinite eddy cascade and, on the other, it must account for the intense mixing and transport properties as the important feature of turbulence.

2. Stochastic turbulence modelling

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

$$F(\boldsymbol{x},t) = \overline{F}(\boldsymbol{x}) + f(\boldsymbol{x},t) \tag{2.1}$$

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

$$\begin{aligned} U_i(\boldsymbol{x}_j,t) &= \overline{U_i}(\boldsymbol{x}_j) + u_i(\boldsymbol{x}_j,t) \\ p(\boldsymbol{x}_j,t) &= \overline{p}(\boldsymbol{x}_j) + p'(\boldsymbol{x}_j,t) \\ \rho(\boldsymbol{x}_j,t) &= \overline{\rho}(\boldsymbol{x}_j) + \rho'(\boldsymbol{x}_j,t) \end{aligned} \tag{2.2}$$

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

$$\rho\Big(\frac{\partial \overline{U_i}}{\partial t} + \overline{U_j}\frac{\partial \overline{U_i}}{\partial x_j}\Big) = \frac{\partial}{\partial x_j}(\sigma_{ij}) + \overline{F_i} \tag{2.3}$$

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

$$\sigma_{ij} = -\overline{p}\delta_{ij} + \nu\rho\Big(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\Big) - \overline{\rho u_i u_j} \tag{2.4}$$

contains an additional term

$$(\sigma_T)_{ij} = -\rho\overline{u_i u_j} \tag{2.5}$$

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

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

represent normal stress components, while the off-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 the Reynolds equations are no longer closed. The closure of the Reynolds equation may be based on a proposal concerning the mutual relation between the Reynolds stress components and physical quantities characterising the mean flow field. Such a concept was proposed by Boussinesq, who introduced a simple linear relation between the Reynolds stress tensor and the mean flow rate of the strain tensor, i.e.

$$-\rho\overline{u_i u_j} = \rho\nu_T\Big(\frac{\partial\overline{U_i}}{\partial x_j} + \frac{\partial\overline{U_j}}{\partial x_i}\Big) \tag{2.6}$$

The proportionality coefficient ν_T, which appears in the above relation is the kinematic turbulent viscosity and may be regarded analogously to Newton's 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 a turbulent flow which depends on the turbulence structure in a given point. The Boussinesq concept enables analytical treatment of a 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 is a scalar quantity, determined experimentally as a function of space coordinates, i.e.

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

which is meant to enable formulation of missing relations between the turbulent stress and the rate of strain tensors. However, such a closure can not be performed for a turbulent flow, because the eddy viscosity is a function of the flow-field which is not *a priori* known. Furthermore, the assumption concerning scalar behaviour of the eddy viscosity was also a matter of serious controversies and as it was pointed out by many authors (e.g. Hinze, 1975). The eddy viscosity should rather be a second order tensor given by the formula

$$-\rho(\overline{u_i u_j}) = (\nu_T)_{ik}\overline{D_{jk}} \tag{2.7}$$

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

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

This improved proposal is, however, not entirely correct because, as it has been pointed out by numerous sources (see for example Elsner, 1987), it does not fulfil the basic assumptions concerning the 3D character of turbulent fluctuations. This limitation may be lifted if Eq. (2.7) is expressed in the form

$$-\overline{u_i u_j} = \frac{1}{2}\{(\nu_T)_{ik}\overline{D_{kj}} + (\nu_T)_{jk}\overline{D_{ki}}\} - \alpha_{ij}k \tag{2.8}$$

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

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

The first term of the r.h.s. of Eq. (2.8) has been written in a form which provides symmetry of the $\overline{u_i u_j}$ tensor indices with respect to i and j. The second term is related to the kinetic turbulence energy and takes into account the presence of normal components of turbulent stresses which have non-zero values even in homogeneous flows where the mean rate of strain tensor is equal to zero. One should notice, however, that introduction of the eddy viscosity expressed as the second order tensor is not a closure of the Reynolds equations but it only illustrates the complexity of the problem.

These closure hypotheses, which have been 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 the $k - \epsilon$ turbulence model developed at the beginning of the 70's and most widely used so far (Launder and Spalding, 1972). 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 of these limitations was the reason why at the very beginning of turbulence modelling era, the idea of stress transport models, which do not use the eddy-viscosity concept, was proposed by Hanjalic (Launder and Spalding, 1972). Stochastic turbulence models were intensively investigated during the 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 (1993) and ending with the recent monography by Pope (2000).

During the 90's the knowledge about turbulence modelling was utilised 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 classical turbulence models solve 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 an extremely successful EU project known under the acronim QNET-CFD (2000).

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 have not resulted in the development of a truly universal turbulence model (Shah and Ferziger, 1997), and unfortunately a pessimistic forecast of Ferziger (1977) formulated as early as at the end of the 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 we use now as the closure for the 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 to find a new solution, which could bring a real breakthrough in CFD and propose a trustworthy description of turbulent flows (Rodi *et al.*, 1997).

3. New perspectives for deterministic turbulence modelling

The research performed during the 90's revealed that, contrary to previous expectations, the N-S equations are capable to describe correctly the structure of turbulent flows in ranges of Reynolds and Mach numbers which are potentially interesting from the engineering point of view. As it was stated by Lesieur (1990), there are simple, good quality solutions to N-S equations for very high Mach numbers ($\mathrm{Ma} \approx 15$), 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 to one knows the initial positions and velocities of all scales of motion, then there should be only one possible state of flow for every time instant* $t > t_0$*."*

From the point of view of a mathematician, this question concerns the problem of existence and uniqueness of a solution to the N-S equation, which so far has only been proved for 2D space (Temam, 1977), while in 3D the N-S solution exists only for a finite time. There seems to be however, a reasonably justified hope (see Lesieur (1990) among others) that the presence of viscosity in the N-S equation will tend to "smooth" the solution at a degree which will be sufficient to prevent singularities and bifurcations to another solution (Iooss and Joseph, 1980).

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

The next advantage of the DNS method is its ability to correctly reproduce 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 the macroscopic flow dimension is of the order

$$L = \frac{\sqrt{k^3}}{\varepsilon} \tag{3.1}$$

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

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

$$\eta = \frac{\nu^3}{\varepsilon} \tag{3.2}$$

The turbulence is inevitably a 3D phenomenon, so if one takes into account relations (3.1) and (3.2), then the number of grid nodes needed for a correct DNS solution may be evaluated as

$$N_{DNS} \approx \mathrm{Re}^{9/4} \tag{3.3}$$

For typical technical applications, the Re number based on turbulence macroscale is of the order of 10^4-10^6, and for geophysical flows it may be even as large as 10^7-10^8, so the number of nodes calculated from Eq. (3.3) is enormous and the same is the size of computer memory needed for the accurate DNS solution. The most powerful computers, which exist nowadays, enable one to obtain DNS solutions for turbulent flows characterised by Re numbers

$$\mathrm{Re} \approx 10^3$$

which is certainly not sufficient for most practical applications. Summing up, DNS is the most promising perspective in research aimed at 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 the 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 (Smagorinsky, 1963), was for the first time successfully applied to industrial flows as early as in 1970 (Deardorff, 1970). The basic assumption of the LES method is separation of the continuous spectrum of eddy scales into resolved (i.e. computed) and modelled scales. It means that turbulent flow quantities like velocity, pressure, etc. are computed for scales comparable to the mesh size of the computational grid, while the same quantities resulting from scales smaller than the mesh size are being modelled. This assumption correctly reflects one of the basic features of turbulence, i.e. the tendency towards isotropy in small scales, which allows one 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 solutions, provided of course that a properly universal subgrid turbulence model may be found.

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

$$\overline{\overline{F}}(\boldsymbol{x}) = G(\boldsymbol{x}) * F(\boldsymbol{x}) = \int\limits_{-\infty}^{+\infty} G(x-\xi)F(\xi)\, d\xi \tag{4.1}$$

where the symbols $(\bar{\bar{\cdot}})$ and $*$ denote the result of the filtration and convolution operators, respectively.

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

$$\frac{\partial \overline{\overline{U}}_i}{\partial t} + \frac{\partial(\overline{\overline{U}}_i \cdot \overline{\overline{U}}_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{\overline{p}}}{\partial x_i} + \frac{\partial}{\partial x_j}\Big[\nu\Big(\frac{\partial \overline{\overline{U}}_i}{\partial x_j} + \frac{\partial \overline{\overline{U}}_j}{\partial x_i}\Big) - \tau_{ij}\Big] \tag{4.2}$$

where one may notice the appearance of the so-called subgrid stress tensor τ_{ij} which is given by the formula

$$\tau_{ij} = \overline{\overline{U_i U_j}} - \overline{\overline{U_i}} \cdot \overline{\overline{U_j}} \tag{4.3}$$

The results obtained by Ferziger and Vreman (Ferziger, 1977; Vreman *et al.*, 1997) reveal that the subgrid turbulence contains 20-30% of the 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 the subgrid turbulence is certainly larger than in the case of the classical RANS approach.

The first reviews of the state-of-art in the field of subgrid modelling have been recently given by Domaradzki and Saiki (1997), Lesieur and Metais (1996) as well as by Jimenez and Moser (2000). 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 and Saiki (1997), who distinguished three main groups of subgrid models, i.e.:

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

The viscosity-based models utilise the Boussinesq (Lesieur and Metais, 1996) concept, transformed as follows

$$\tau_{ij} = \nu_t S_{ij} + \frac{1}{3}\tau_{ll} S_{ij} \tag{4.4}$$

where τ_{ij} denotes the subgrid stress tensor given by Eq. (4.3), ν_t is the subgrid eddy viscosity coefficient, while the expression

$$S_{ij} = \frac{\partial \overline{\overline{U_i}}}{\partial x_j} + \frac{\partial \overline{\overline{U_j}}}{\partial x_i} \tag{4.5}$$

is the rate of the strain tensor of the filtered flow field. The first subgrid closure was proposed by Smagorinsky (1963), who developed a subgrid analogy to the mixing length model, given by the following formula

$$\nu_t = (C_s \varDelta)^2 |S| \tag{4.6}$$

where $\varDelta$ denotes the characteristic subgrid length scale (or filter width), C_s is a constant adjusted arbitrarily for a given flow type (solution), while the absolute measure of local strain is given by the formula

$$|S| = \sqrt{2 S_{ij} S_{ij}} \tag{4.7}$$

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's models reveal also some serious limitations. First of all, one should mention among them too large value of the subgrid eddy viscosity $\overline{\nu_t}$ in the vicinity of walls, which requires using of some correcting functions. Furthermore, it is difficult to propose a sound physical explanation for the proper value of the characteristic subgrid length scale $\varDelta$, see Eq. (4.6), and that is why this important parameter has to be selected in an arbitrary manner. Finally, Smagorinsky's model is unable to correctly predict 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 were proposed. Among the most successful proposals and improvements of the original Smagorinsky idea, the following seem to be the most valuable:

- Structure Function Model by Metais and Lesieur (1992)
- Selective Structure Function Model by David (1993)
- Filtered Structure Function Model developed by Ducros (1995).

One should also notice a group of models based on spectral formulation by Kraichnan (1976), which are discussed in more detail in Lesieur (1990), Lesieur and Metais (1996) as well as an interesting generalisation of the Smagorinsky model, which was presented as the HS (Hyper Smagorinsky) model by Jimenez and Moser (2000).

Mixed models have been originally proposed by a famous research group at Stanford University (Bardina *et al.*, 1983), and this type of closure together with the dynamic model proposed by Germano *et al.* (1991) are not models in the traditional sense. In fact, both mixed and dynamic models are rather complex algorithms which try to relate subgrid stresses with scales of resolved motion (Tyliszczak, 1998).

The variety of subgrid models developed so far is, on one hand, a proof of the importance of this branch of CFD, but on the other, 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 the turbulence structure for various flow types. Nevertheless, both the older (Rogallo and Moin, 1984) and the more recent (Ferziger, 1996; Härtel, 1996) reviews on the subject prove that subgrid modelling is still the key issue for further development of the LES technique.

5. Summary

A brief description of current trends in the modelling of turbulence proves the important role of the deterministic approach. Both DNS and LES techniques do not, however, continue the trends developed by the traditional RANS modelling, but in fact both these approaches are novel treatments of the 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 the LES, which presents a reasonable compromise between the accuracy of solution and demand for computational effort.

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Uwagi o modelowaniu i symulacji turbulencji

Streszczenie

Praca przedstawia współczesny stan wiedzy w dziedzinie numerycznego modelowania turbulencji ze szczególnym uwzględnieniem metody LES (ang. *Large Eddy Simulation*). Przedstawiono ograniczenia modeli turbulencji typu RANS, opartych o uśrednione w czasie równania Reynoldsa oraz wskazano perspektywy deterministycznego ujęcia turbulencji z użyciem metod DNS (ang. *Direct Numerical Simulation*). Wykazano również, że możliwości najszybszych dostępnych obecnie komputerów ograniczają możliwe obszary aplikacji DNS do przepływów o stosunkowo niskich liczbach Reynoldsa. Następnie sformułowano podstawowe zależności dla metod LES i wskazano ich perspektywiczne znaczenie dla inżynierskiego modelowania przepływów turbulentnych.

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